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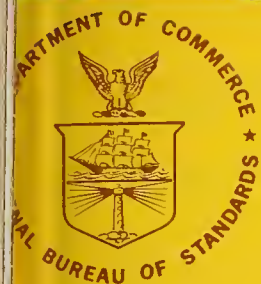
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PUBLICATIONS

NAT'L INST OF STANDARDS & TECH R.I.C.



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NBS MONOGRAPH 25— SECTION 14

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Standard X-ray Diffraction Powder Patterns

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No.25-14
1977
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¹ Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.

² Located at Boulder, Colorado 80302.

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Standard X-ray Diffraction Powder Patterns Section 14—Data for 68 Substances

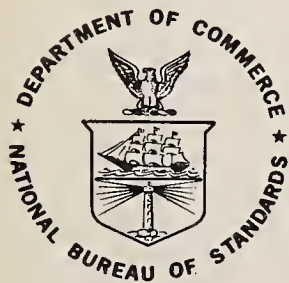
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Joint Committee on
Powder Diffraction Standards

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ERRATA

A book has been published containing card images of NBS Standard X-ray Diffraction Powder Patterns¹. During preparation of the book, some errors were found and corrected on the card images. A list of them is available on request. The corrections below are in addition to those included on the card images.

Circular 539

- Vol. 1, p. 67 Density should be 2.749 g/cm³
 1, p. 78 In the test for chemical analysis, the word should be "thiocyanate."
 2, p. 28 Previous erratum (Mono. 25, Sec. 5) changed the space group to Ia3. Change also the following indices: for d = 2.068, 1.808, 1.491, 1.1646, and 1.1110, use hkl = 431, 433, 543, 833, and 851 respectively.
 3, p. 27 Previous erratum (Mono. 25, Sec. 5) changed the space group to Ia3. Change also the following indices: for d = 1.9301, 1.6885, and 1.3924, use hkl = 431, 433, and 543 respectively.
 4, p. 67 In the lattice constants, the NBS values for "b" and "c" should be interchanged. Because "b" and "c" are so nearly equal, a few indices may also need to be changed.
 5, p. 30 At hkl = 321, "d" should be 1.4479. At hkl = 631, "d" should be 0.7987.
 6, p. 41 Delete "CdI₂-type structure." Insert "K₂GeF₆ is used as a structure type."
 10, p. 4 Formula in title should be AlPO₄.

Monograph 25

- Sec. 5, p. 11 At hkl = 002, d should be 4.401.
 11, p. 39 Add this structural information: "The cubic cell given with Z = ½ is a pseudo-cell. The true cell with Z = 1 has random voids in the Hg position."
 12, p. iii The formula for magnesium titanium oxide should be Mg₂TiO₄.
 12, p. 42 The text and the references at the end should both have the year 1975 for the reference to McMurdie et al.
 13, p. 26 At d = 1.648, the hkl's should be 442, 530.
 13, p. 36 At d = 2.423, the intensity should be 20.
 13, p. 79 Density should be 8.605.

¹Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976). (The Joint Committee on Powder Diffraction Standards, Swarthmore, PA, 19081, \$150.00).

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

The following copies may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, Virginia, 22161. Where these publications are identified with a number, it must be used in ordering. They are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

Also, until the present supply is exhausted, the publication numbers marked by an asterisk are for sale from the Superintendent of Documents, U. S. Government Printing Office, Washington, D. C. 20402. Order Sections 11, 12, and 13 respectively, by catalog no. SN 003-003-01234-3, \$1.55; SN 003-003-01376-5, \$1.50; or C13.44:25/Sec. 13, \$1.80. (Add 25% additional for other than U. S. mailing).

NBS Publication	Number	NBS Publication	Number
Circular 539, Volume 1.....	PB 178 902	Monograph 25, Section 1.....	PB 178 429
Volume 2.....	PB 178 903	Section 2.....	PB 178 430
Volume 3.....	PB 178 904	Section 3.....	PB 178 431
Volume 4.....	PB 178 905	Section 4	
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Volume 6.....	PB 178 907	Section 6	
Volume 7.....	PB 178 908	Section 7	
Volume 8.....	PB 178 909	Section 8.....	PB 194 872
Volume 9.....	PB 178 910	Section 9.....	COM 72-50002
Volume 10.....	PB 178 911	Section 10.....	COM 72-51079
		*Section 11.....	COM 74-50183
		*Section 12.....	COM 75-50162
		*Section 13.....	

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 14. --- Data for 68 Substances

by

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Boris Paretzkin, and Johan H. de Groot
Assisted by Rainer J. Newberry*
Joint Committee on Powder Diffraction Standards

and

Camden R. Hubbard and Simon J. Carmel
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Standard x-ray diffraction patterns are presented for 68 substances. Twenty-seven of these patterns represent experimental data and 41 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

Key words: Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the Joint Committee on Powder Diffraction Standards,¹ the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the Joint Committee, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 68 compounds (27 experimental and 41 calculated patterns), and is the twenty-fourth of the series of "Standard X-ray Diffraction Powder Patterns."²

EXPERIMENTAL POWDER PATTERNS

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the sample improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

Optical data. In some cases, optical measurements were made by grain immersion methods, in white light, using oils standardized in sodium light, in the refractive index range 1.49 to 2.1 [Hartshorne and Stuart, 1970].

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard (approximately 5 wt. percent tungsten powder). If tungsten lines were found to interfere with sample lines, silver or silicon was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used. To avoid errors associated with aberrations at the very top of peaks, the readings of 2 θ were taken at positions about 20 percent of the way down from the top, and in the center of the peak width. The internal standard correction for each region was then applied to the measured value of 2 θ . We have reported all data as $K\alpha_1$ peaks because the internal standard corrections for all regions were established in terms of the $K\alpha_1$ wavelength.

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¹Joint Committee on Powder Diffraction Standards, 1601 Park Lane, Swarthmore, PA. 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

²See previous page for other published volumes.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in the table below; the 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Calculated 2θ Angles, $\text{CuK}\alpha_1$ $\lambda = 1.540598\text{\AA}$			
hkl	W a=3.16524 \AA ± 0.00004	Ag a=4.08651 \AA ± 0.00002	Si a=5.43088 \AA ± 0.00004
110	40.262		
111		38.112	28.443
200	58.251	44.295	
211	73.184		
220	86.996	64.437	47.303
310	100.632		
311		77.390	56.123
222	114.923	81.533	
321	131.171		
400	153.535	97.875	69.131
331		110.499	76.377
420		114.914	
422		134.871	88.032
511/333		156.737	94.954
440			106.710
531			114.094
620			127.547
533			136.897
444			158.638

The new internal standard Si powder is available as Standard Reference Material 640 [1974]. The lattice constant for the Si was refined from multiple powder data measurements made with tungsten as an internal standard [Swanson et al., 1966]. Cell parameter data were also collected for a single crystal from the boules ground to prepare the powder. The lattice parameters from the two methods agreed within 3 parts in 10^5 [Hubbard et al. 1975]. D-spacing results using SRM 640 will be in agreement with patterns recorded in this series of monographs since 1966.

All of our spacing measurements were recorded at 25 ± 1 °C on a diffractometer equipped with a focusing graphite or lithium fluoride crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. All measurements were performed using copper radiation: $\lambda(\text{CuK}\alpha_1, \text{peak}) = 1.540598\text{\AA}$ [Deslattes and Henins, 1973].

Structure, lattice constants. The space groups were listed with short Hermann-Mauguin symbols as well as the space group numbers given in the *International Tables for X-ray Crystallography*, Vol. I [1952].

Orthorhombic cell dimensions were arranged according to the Dana convention $b > a > c$ [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary in order to follow the convention of *Crystal Data* [1973]. For primitive cells, the transformed cell axes are an alternate labelling of the reduced cell

axes. For centered monoclinic cells, the transformed cell is the centered cell with the three shortest non-coplanar vectors.

A computer program [Evans et al., 1963] assigned hkl's and refined the lattice constants. Cell refinement was based only upon $2\theta_{\text{obs}}$ values which could be indexed without ambiguity. The program minimized the value $\sum(\theta_{\text{obs}} - \theta_{\text{calc}})^2$. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. In indexing cubic patterns, multiple hkl's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest h was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943×10^{23} [Deslattes et al., 1974] and atomic weights published by IUPAC [1972].

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than $10\text{ }\mu\text{m}$, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical





position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (as shown in Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line. Any intensity larger than 20 was rounded to the nearer multiple of 5. At least 3 patterns for intensity measurements were prepared for each sample to check reproducibility.

Reference Intensity Ratio, I/I_{corundum} . The reference intensity ratio, I/I_c , has been defined as the direct ratio of the intensity of the strongest reflection of a sample, to the intensity of the reflection 113(hexagonal) of corundum [Visser and de Wolff, 1964]. The ratio is tabulated for copper $K\alpha$ radiation, for a 1:1 mixture by weight of the sample and corundum.

A new procedure has been adopted, to achieve greater statistical accuracy [Hubbard and Smith, 1977]. For any weight fractions of sample and corundum, x_s and x_c ($x_s = 1 - x_c$), intensities $I(h)$ and $I(k)$ are measured for several sets of reflections h and k , usually within the same region of 2θ , to provide indications of possible preferred orientation, extinction, or other systematic errors. The reference intensity ratio is then given by

$$\frac{I(h_0)}{I_c(113)} = \frac{x_c}{x_s} \cdot \frac{I_c^{\text{rel}}(k)}{I_c^{\text{rel}}(h)} \cdot \frac{I(h)}{I(k)}$$

and (h_0) indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection (h_0) will be the one with $I=100$ since only copper radiation was used. Typically, at least 3 sets of reflections and 2 mountings of the mixture were used to obtain 6 or more values for the reference intensity ratio, I/I_c . These values yield the tabulated average

$\langle I/I_c \rangle$. From these data, an estimated standard deviation, Δ , (given in parentheses), was obtained from

$$\Delta = \frac{\sum_{i=1}^n |(I/I_c)_i - \langle I/I_c \rangle|}{n}$$

where n is the number of measurements of the reference intensity ratio.

CALCULATED POWDER PATTERNS

Since some substances of interest are not readily available for experimental work, powder patterns were calculated from published crystal structure data. The FORTRAN program used for the computations was developed by Clark, Smith and Johnson [1973] and modified at NBS.

Lattice parameters. Before the computations of the patterns, any necessary changes were made in the lattice constants in order to make them consistent with the revised value of $\lambda(\text{CuK}\alpha_1) = 1.540598\text{\AA}$ [Deslattes and Henins, 1973]. Both the altered and the original published values are given. A lattice constant arrangement which follows the conventions of Crystal Data has been referred to as the "CD cell." In several of the calculated patterns, the literature lattice constants, the atom positions, and hence the final patterns were not given in the CD arrangement. For cross-reference purposes, the CD cell was calculated separately and included in the text.

Scattering factors. Whenever possible, the same scattering factors were used which the author of the reference article specified. Otherwise, the factors were taken directly from the *International Tables for X-ray Crystallography*, Vol. III, [1962]. The factors were corrected for dispersion if the author had done so.

Thermal parameters. The computer program used thermal parameter data of only two forms, the isotropic B 's or the anisotropic β_{ij} 's in the following expressions:

$$e^{(-B \sin^2\theta)/\lambda^2}$$

or

$$e^{-(h^2\beta_{11} + k^2\beta_{22} + \ell^2\beta_{33} + 2hk\beta_{12} + 2h\ell\beta_{13} + 2k\ell\beta_{23})}.$$

Other thermal parameters were converted to one of these two forms. The isotropic parameters were used directly, if given by the structure reference. In a few of our patterns, anisotropic parameters were also used directly as given by the structure reference; in other work, instead of using given anisotropic parameters, approximately equivalent isotropic values were substituted as defined by:

$$B = 4 \left[\frac{\beta_{11}\beta_{22}\beta_{33}}{a^2 b^2 c^2} \right]^{\frac{1}{3}}$$

Structural information. The atom positions used in these calculated patterns varied somewhat in the degree of reliability. In our text, when the expression "the structure was determined by..." was used, the atomic parameters in the reference cited had been calculated from refinement of single crystal data. Otherwise, the atomic positions had been derived by analogy with similar compounds whose structure was known. In cases where isostructural relationships were used, the atoms were in fixed special positions or the ionic radii were closely related to the corresponding radii of the atoms in the known structure.

Integrated intensities. The theoretical integrated intensity of reflection i on the "absolute/relative" scale is computed from the right hand side of the equation:

$$\frac{I_i^{abs}}{K} = \frac{M_i L_p |F_i T_i|^2}{2\mu V^2}$$

where:

F is the structure factor
 T is the thermal correction

$L_p = \frac{1+\cos^2 2\theta}{\sin^2 \theta \cos \theta}$ is the Lorentz-polarization term

M is the multiplicity for the reflection i
 μ is the linear absorption coefficient
 V is the volume of the unit cell

When the largest integrated intensity was assigned a relative value of 100 and all other reflections were scaled relative to it, the intensities were placed on the relative intensity scale (I^{rel}). Relative intensities were rounded to the nearest integer value before being listed, and reflections with I^{rel} less than 0.7 were omitted.

Scale factor (integrated intensities). The scale factor, γ , was defined to convert the tabulated I^{rel} to the "absolute/relative" scale [Hubbard, Evans and Smith, 1976]. That is:

$$\gamma = \frac{M' L_p' |F' T'|^2}{200\mu V'^2}$$

and

$$\frac{I_i^{abs}}{K} = \gamma I_i^{rel}$$

The primes denoted the values for the largest integrated intensity. In earlier Monographs (1969-1975), a different scale factor, k_{NBS} , was reported which is related to γ :

$$\frac{\gamma}{k_{NBS}} = \frac{1}{2\mu V'^2}$$

From γ , the theoretical value of the Reference Intensity Ratio, I/I_c , was calculated:

$$I/I_c = \frac{\mu \gamma \rho_c}{\mu_c \gamma_c \rho}$$

where ρ is the density and the subscript c represents corundum (α - Al_2O_3).

For refined structures, the value of I/I_c was given. For those phases whose structures were postulated or were based only on analogy to other powder patterns, I/I_c was not included and any intensity above 20 was rounded further, to the nearer multiple of 5.

I/I_c and γ are each based on the single strongest reflection, not on the overlapping sum of superimposed reflections.

Peak intensities. The purpose of calculating peak intensities was to provide a tabulated pattern similar to what might be obtained from experimental diffractometer measurements. For each predicted reflection, Cauchy profiles centered at both the α_1 and the α_2 peak positions were calculated and summed, forming a simulated powder pattern. The full width at half-maximum (FWHM) was allowed to vary to represent the changing FWHM as a function of 2θ . [The values of the FWHM vs 2θ are given in the table below]. The resultant simulated powder pattern was then analyzed for peaks. In the regions of the predicted reflections several reflections could have identical or similar 2θ angles and produce only one composite peak in the simulated pattern. The 2θ angle of the composite peak was assigned the hkl of the reflection having the greatest contribution to the peak intensity. If any other peak contributed more than 10% of the intensity toward the composite peak intensity, a plus sign (+) was appended to the hkl . Peaks due solely to α_2 lines were omitted. If an α_1 peak and an α_2 peak overlapped, the α_1 reflection was listed only when it contributed a significant intensity (>10%) at the peak 2θ .

The peak search routine located peaks only at 2θ angles which were a multiple of 0.02° .

2θ	FWHM	2θ	FWHM
CuK α_1		CuK α_1	
0°	0.12°	140	0.230
20	.12	145	.255
40	.12	150	.285
60	.125	155	.315
80	.130	160	.360
100	.135	162.5	.410
120	.155	165	.500
130	.185		

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- Palache, C., Berman, H. and Frondel, C. (1944). *Dana's System of Mineralogy* (John Wiley and Sons, New York, 7th Ed.), I, 6.
- Standard Reference Material 640, Silicon Powder, X-ray Diffraction Standard, obtainable from the Office of Standard Reference Materials, Room B311, Chemistry Building, National Bureau of Standards, Washington, D.C. 20234. \$52.00 per 10 gram unit.
- Swanson, H. E., Morris, M. C., and Evans, E. H. (1966). Nat'l Bur. Std. U.S. Monograph 25, Sec. 4, 3.
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Ammonium iron chloride hydrate, $(\text{NH}_4)_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation at room temperature of an acid aqueous solution of NH_4Cl and FeCl_3 .

Color

Deep reddish orange

Optical Data

Biaxial (+), $N_\alpha = 1.755$, $N_\beta = 1.77$, $N_\gamma = 1.82$.
2V is large.

Structure

Orthorhombic, Pmnb (62), $Z=4$, isostructural with $\text{K}_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ (erythrosiderite) [Bellanca, 1947].
The structure of $(\text{NH}_4)_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ was determined by Lindqvist [1946, 1948].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 9.925(3) \text{ \AA} \\ b &= 13.713(3) \\ c &= 7.039(2) \end{aligned}$$

Volume

$$957.9 \text{ \AA}^3$$

Density

$$(\text{calculated}) 1.991 \text{ g/cm}^3$$

Reference intensity

$$I/I_{\text{corundum}} = 0.8$$

References

Bellanca, A., (1947). Ric. Sci. Ricostr. 17, 1360.
Lindqvist, I., (1946). Ark. Kemi Mineral. Geol. A24, No. 1.
Lindqvist, I., (1948). Acta Chem. Scand. 2, 530.

$$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}; \text{ temp. } 25 \pm 1 \text{ }^\circ\text{C}$$

$$\text{Internal standard Ag, } a = 4.08651 \text{ \AA}$$

d(Å)	I	hkl	2θ(°)
6.26	8	011	14.13
5.74	100	101	15.43
5.64	95	120	15.71
5.29	9	111	16.73
4.96	60	200	17.87
4.92	80	021	18.03
4.39	5	121	20.19
4.01	6	220	22.13
3.836	12	031	23.17
3.579	5	131	24.86
3.515	5	002	25.32
3.492	4	221	25.49
3.426	6	040	25.99
3.410	4	012	26.11
3.082	17	041	28.95

d(Å)	I	hkl	2θ(°)
3.034	18	231	29.42
2.989	25	122	29.87
2.983	25	320	29.93
2.945	12	141	30.32
2.869	35	202	31.15
2.820	95	240	31.70
2.812	85	212	31.80
2.787	65	032	32.09
2.742	4	321	32.63
2.685	5	132	33.34
2.648	5	222	33.83
2.617	4	241	34.24
2.557	4	051	35.07
2.481	65	400	36.17
2.456	50	042	36.55
2.432	4	232	36.93
2.382	5	142, 340	37.73
2.313	11	013	38.91
2.308	9	411	38.99
2.227	4	160	40.47
2.214	20	421	40.73
2.202	12	242	40.96
2.174	11	061	41.50
2.163	15	052	41.73
2.114	13	152	42.73
2.082	11	431	43.42
2.042	19	133	44.32
1.991	6	261	45.53
1.984	4	252	45.68
1.932	7	441	46.99
1.907	10	520	47.66
1.881	8	162, 360	48.34
1.854	25	171, 432	49.10
1.811	6	352	50.34
1.782	7	053	51.22
1.764	5	271	51.78
1.745	25	442, 014	52.40
1.7180	13	540	53.28
1.7150	8	512, 080	53.38
1.6915	8	413	54.18
1.6696	6	541	54.95
1.6654	5	081	55.10
1.6429	8	181, 034	55.92
1.6346	8	461	56.23
1.6304	9	452	56.39
1.6201	6	280, 134	56.78
1.5434	5	542, 314	59.88

Ammonium potassium iron chloride hydrate, (kremersite) $(\text{NH}_4, \text{K})_2 \text{FeCl}_5 \cdot \text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation at room temperature of a 1:1:1 molar aqueous solution of NH_4Cl , KCl and FeCl_3 . The first crystals formed were used. From a plot of the cell parameters of the end members of the solid solution series, this sample was determined to be close to a 1:1 molar ratio of NH_4 to K. This is similar to the reported analysis of the natural mineral, kremersite, from Mt. Vesuvius [Palache et al., 1951].

Color

Deep reddish orange

Structure

Orthorhombic, Pmnb (62), $Z=4$, isostructural with $\text{K}_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ and $(\text{NH}_4)_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$. The structure of $\text{K}_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ was determined by Bellanca [1947].

NBS lattice constants of this sample

$a = 9.808(3) \text{ \AA}$
 $b = 13.657(4)$
 $c = 7.028(2)$

Volume

941.4

Density

(calculated) 2.175 g/cm^3 .

Reference Intensity

$I/I_{\text{corundum}} = 1.2$

References

Bellanca, A. (1947). *Ric. Sci. Ricostr.* **17**, 1360.
 Palache, C., Berman, H., and Frondel, C. (1951). *Dana's System of Mineralogy* (John Wiley & Sons, New York, 7th Ed.) pg. 101.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard Si, $a = 5.43088 \text{ \AA}$			
$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
5.72	80	101	15.48
5.61	55	120	15.78
5.270	7	111	16.81
4.900	40	200,021	18.09
3.820	6	031	23.27
3.464	7	221	25.70
3.411	9	040	26.10
3.070	16	041	29.06
3.016	17	231	29.60
2.966	13	301	30.11
2.951	9	320	30.26
2.857	25	202	31.28
2.800	100	240	31.93
2.794	60	212	32.00
2.783	55	032	32.14
2.601	4	241	34.45
2.548	3	051	35.20
2.451	65	400,042	36.64
2.374	4	142	37.86
2.310	4	013	38.95
2.277	2	060	39.54
2.191	11	421,242	41.16
2.157	12	052	41.84
2.106	9	152	42.91
2.038	14	133	44.41
1.889	7	501	48.14
1.839	15	432	49.54
1.800	4	352	50.66
1.798	2	243	50.74
1.779	4	053	51.33
1.742	7	014	52.49
1.7327	13	442	52.79
1.6585	4	081	55.35
1.6541	3	204	55.51
1.6193	6	452	56.81

Ammonium strontium chromium oxide, $(\text{NH}_4)_2\text{Sr}(\text{CrO}_4)_2$

Sample

The sample was precipitated by adding a strong solution of SrCl_2 to one of $(\text{NH}_4)_2\text{CrO}_4$, following the method of Schwarz [1966]. This material gave somewhat broad peaks which suggest that the compound may be of lower symmetry.

Color

Dark orange yellow

Structure

Hexagonal, $R\bar{3}m(166)$, $Z = 3$, isostructural with $\text{Sr}_3(\text{PO}_4)_2$ and many other double chromates and sulfates [Schwarz, 1966]. The structure of $(\text{NH}_4)_2\text{Pb}(\text{SO}_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

$$a = 5.758(1) \text{ \AA}$$

$$c = 22.027(4)$$

Volume

$$632.3 \text{ \AA}^3$$

Density

(calculated) 2.802 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 2.2(3)$$

Additional pattern

1. PDF card 19-70 [Schwarz, 1966].

References

Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 345, 230.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
7.345	60	003	12.04
4.868	5	101	18.21
4.546	45	012	19.51
3.696	10	104	24.06
3.672	6	006	24.22
3.300	100	015	27.00
2.881	60	110	31.02
2.680	30	113	33.41
2.662	13	107	33.64
2.434	4	202	36.90
2.411	2	018	37.26
2.271	8	024	39.65
2.266	9	116	39.75
2.169	20	205	41.61
2.015	20	1•0•10	44.95
1.955	2	027	46.42
1.857	6	0•1•11,122	49.01
1.848	11	208	49.26
1.836	6	0•0•12	49.61
1.783	2	214	51.19
1.732	11	125	52.81
1.662	6	300	55.23
1.651	5	0•2•10	55.63
1.619	4	303,217	56.81
1.604	3	1•0•13	57.40
1.554	2	128	59.41
1.5481	2	1•1•12	59.68
1.4682	3	0•0•15	63.29
1.4392	5	220	64.72
1.4319	11	2•1•10	65.09

Barium vanadium oxide, Ba₃(VO₄)₂

Sample

Prepared by heating stoichiometric amounts of BaCO₃ and V₂O₅ at 825 °C, regrinding and re-heating at 860 °C for 1½ hours, grinding again and heating on Méker burner (~1100 °C) for 10 minutes to improve crystallization.

Color

Colorless

Structure

Hexagonal, R $\bar{3}$ m(166), Z = 3, isostructural with Sr₃(PO₄)₂. The structure was determined by Zachariasen [1948] and refined by Süssé and Buerger [1970].

NBS lattice constants of this sample:

$$a = 5.7845(2) \text{ \AA}$$

$$c = 21.317(1)$$

Volume

$$617.73 \text{ \AA}^3$$

Density

(calculated) 5.176 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 4.7(4)$$

Additional patterns

1. PDF card 19-144 [Lubin & Rittershaus, Gen'l. Tel. and Electronics, N.Y. (1966)].
2. PDF card 25-1192 [Smith et al., 1974].
3. Zachariasen [1948].

References

- Smith, D. K., et al., (1974). Annual Report to the Joint Committee on Powder Diffraction Standards.
- Süssé, P., and Buerger, M. J., (1970). Z. Kristallogr. 131, 161.
- Zachariasen, W. H., (1948). Acta Crystallogr. 1, 263.

CuK α ₁ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkl	2 θ (°)
7.09	4	003	12.47
4.878	11	101	18.17
4.537	3	012	19.55
3.651	12	104	24.36
3.247	100	015	27.45
2.893	75	110	30.88
2.487	4	021	36.09
2.439	7	202	36.82
2.369	9	009	37.95
2.353	3	018	38.22
2.267	11	024	39.72
2.243	6	116	40.17
2.160	40	205	41.79
1.962	25	1·0·10	46.24
1.934	4	027	46.95
1.886	3	211	48.20
1.833	10	119	49.71
1.785	3	214	51.14
1.731	25	125	52.85
1.670	13	300	54.92
1.624	12	0·2·10	56.64
1.543	1	128	59.90
1.511	2	306	61.30
1.457	4	0·1·14	63.85
1.446	10	220	64.38
1.421	4	0·0·15	65.66
1.416	13	2·1·10	65.92
1.386	1	131	67.53
1.3647	3	309	68.73
1.3445	1	134	69.91
1.3208	9	315	71.35
1.3010	2	2·0·14	72.61
1.2755	10	1·1·15	74.30
1.2438	1	042	76.53
1.2343	4	229	77.23
1.2324	2	318	77.37
1.2015	4	045	79.75
1.1864	3	1·2·14	80.97
1.1641	5	1·3·10	82.86
1.1235	1	324	86.57
1.1096	5	235	87.93
1.0947	4	1·0·19	89.44
1.0933	5	410	89.59
1.0824	6	3·0·15	90.74
1.0799	5	4·0·10	91.01
1.0425	3	0·1·20	95.27
1.0264	2	3·1·14	97.27
1.0239	2	0·2·19	97.57
1.0135	5	2·2·15	98.93
1.0114	7	3·2·10	99.22

Barium vanadium oxide, $\text{Ba}_3(\text{VO}_4)_2$ - (continued)

CuK α_1 λ = 1.540598 Å; temp. 25±1 °C			
Internal standard W, a = 3.16524 Å			
d(Å)	I	hkl	2 θ (°)
0.9927	2	419	101.78
.9809	2	2•0•20	103.49
.9753	2	505	104.34
.9653	4	2•1•19	105.87
.9641	4	330	106.06
.9288	4	1•2•20	112.07
.9242	3	425	112.91
.9174	2	2•3•14	114.21
.9067	2	0•5•10	116.32
.8802	2	155	122.12
.8729	1	1•3•19	123.87
.8665	1	4•1•15	125.50

Calcium iodate (lautarite), $\text{Ca}(\text{IO}_3)_2$

Sample

The preparation was begun by adding an aqueous solution of $\text{Ca}(\text{NO}_3)_2$ to one of HIO_3 to precipitate $\text{Ca}(\text{IO}_3)_2 \cdot 6\text{H}_2\text{O}$ which was then heated at 160°C . for six hours. It was heated again in a sealed glass tube at 240°C for several hours.

Color

Colorless

Structure

Monoclinic, $\text{P}2_1/\text{n}(14)$, $Z=4$, distorted perovskite type. [Gossner and Mussnug, 1930]. The structure was determined by Gossner, [1937].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 7.280(1) \text{ \AA} \\ b &= 11.304(2) \\ c &= 7.148(1) \\ \beta &= 106.36(2)^\circ \end{aligned}$$

Volume

$$564.4 \text{ \AA}^3$$

Density

(calculated) 4.588 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 2.45(4)$$

Additional Patterns

- PDF card 1-386, labeled $\text{Ca}(\text{IO}_3)_2$ but data is for $\text{Ca}(\text{IO}_3)_2 \cdot \text{H}_2\text{O}$, brüggenite.

References

Gossner, B., (1937). Z. Krist. 96, 381.
Gossner, B., and Mussnug, F., (1930). Z. Krist. 75, 410.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ\text{C}$			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
d(Å)	I	hkl	2 θ (°)
5.93	12	110	14.93
5.866	5	011	15.09
5.779	5	$\bar{1}01$	15.32
5.651	3	020	15.67
5.139	5	$\bar{1}11$	17.24
4.360	50	021	20.35
4.037	17	$\bar{1}21, 111$	22.00
3.493	65	200	25.48
3.428	85	002	25.97
3.378	14	$\bar{2}11$	26.36

d(Å)	I	hkl	2 θ (°)
3.336	40	$210, \bar{1}12$	26.70
3.318	30	130	26.85
3.156	100	$\bar{1}31$	28.25
3.001	18	$\bar{2}21$	29.75
2.931	3	022	30.47
2.885	20	$\bar{2}02$	30.97
2.840	35	131	31.48
2.795	13	$\bar{2}12$	31.99
2.726	10	211	32.83
2.703	4	112	33.12
2.619	2	140	34.21
2.582	2	$\bar{2}31$	34.71
2.560	6	$230, \bar{1}32$	35.02
2.515	8	221	35.67
2.328	2	$\bar{1}13$	38.65
2.292	5	$\bar{2}32$	39.27
2.252	2	231	40.01
2.240	2	$013, 132$	40.22
2.227	8	$\bar{3}21$	40.48
2.199	5	$\bar{3}12$	41.01
2.194	5	$\bar{1}23$	41.11
2.161	18	202	41.77
2.151	8	150	41.97
2.146	5	051	42.06
2.122	5	212	42.57
2.120	5	023	42.64
2.067	3	$\bar{2}23$	43.77
2.038	20	$\bar{3}31, 301$	44.42
2.012	30	$\bar{1}33, 103$	45.02
1.987	4	$330, 113$	45.75
1.926	4	$\bar{3}03$	47.16
1.917	6	321	47.39
1.897	9	$\bar{1}52, \bar{3}13$	47.91
1.884	9	060	48.27
1.840	3	$\bar{3}41$	49.51
1.817	12	061	50.17
1.797	12	340	50.77
1.793	14	331	50.90
1.775	15	133	51.44
1.756	12	$\bar{3}42, 152$	52.05
1.7500	11	$\bar{4}12$	52.23
1.7460	11	$\bar{2}43, \bar{2}04$	52.36
1.7255	11	$410, \bar{2}14$	53.03
1.7138	14	$\bar{3}33$	53.42
1.6863	4	213	54.36
1.6629	7	$\bar{2}61$	55.19
1.6582	8	$260, \bar{1}62$	55.36
1.6514	6	062	55.61
1.6078	1	053	57.25
1.5911	4	$\bar{3}52, \bar{3}43$	57.91
1.5836	4	$\bar{2}53, \bar{2}34$	58.21
1.5780	5	$\bar{2}62$	58.44
1.5735	5	$170, 411$	58.62
1.5645	4	261	58.99
1.5602	4	$034, 162$	59.17
1.5293	1	$441, 421$	60.49

Calcium iodate hydrate, $\text{Ca}(\text{IO}_3)_2 \cdot 6\text{H}_2\text{O}$

Sample

The sample was prepared by adding an aqueous solution of $\text{Ca}(\text{NO}_3)_2$ to one of HIO_3 . The loss in weight at 160°C indicated that it was a hexahydrate.

Color

Colorless

Optical Data

Biaxial, $N_\alpha = 1.604$, $N_\beta = 1.644$, $N_\gamma = 1.686$, $2V$ is large. [Winchell and Winchell, 1964].

Structure

Orthorhombic, $Fdd2$ (43) from precession patterns [Perloff, 1976]. $Z=6$ (from agreement of experimental and calculated densities).

NBS lattice constants of this sample

$$\begin{aligned} a &= 14.866(3)\text{\AA} \\ b &= 23.015(5) \\ c &= 6.392(1) \end{aligned}$$

Volume \AA^3
2187.1 \AA^3

Density

(calculated) 2.268 g/cm^3

Reference Intensity

$$I/I_{\text{corundum}} = 2.4(3)$$

References

Perloff, A. (1976). Private communication.

Winchell, A. N., and Winchell, H. (1964). The Microscopical Characters of Artificial Inorganic Solid Substances (Academic Press, New York and London) p. 109.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ\text{C}$			
Internal standard W, $a = 3.16524 \text{ \AA}$			
d(\AA)	I	hkl	$2\theta(^{\circ})$
5.75	50	040	15.39
5.69	60	111	15.55
4.65	100	131	19.04
3.86	25	311	23.02
3.714	40	400	23.94
3.625	11	151	24.54
3.538	5	420	25.14
3.489	55	331	25.51
3.406	20	260	26.14
3.121	40	440	28.58

d(\AA)	I	hkl	$2\theta(^{\circ})$
3.078	6	022	28.99
2.983	5	351	29.93
2.936	40	202	30.42
2.878	25	080	31.05
2.867	30	171	31.17
2.842	8	222	31.45
2.676	19	511	33.46
2.669	15	460	33.55
2.616	55	242	34.25
2.544	13	531	35.25
2.517	16	371	35.64
2.455	3	062	36.57
2.370	3	422	37.93
2.343	18	191	38.39
2.331	6	262	38.60
2.275	8	640,480	39.59
2.234	1	442	40.34
2.198	7	2 \cdot 10 \cdot 0	41.03
2.142	3	391	42.15
2.101	15	113	43.02
2.081	9	660	43.43
2.055	11	282	44.03
2.048	8	462	44.18
2.034	12	133	44.51
2.007	5	711	45.14
1.971	11	1 \cdot 11 \cdot 1	46.02
1.956	7	4 \cdot 10 \cdot 0	46.38
1.951	19	313,731	46.52
1.930	6	622	47.05
1.917	1	0 \cdot 12 \cdot 0,153	47.39
1.896	4	333	47.95
1.868	9	0 \cdot 10 \cdot 2	48.71
1.853	25	642,482	49.12
1.846	20	751,3 \cdot 11 \cdot 1	49.33
1.802	2	353	50.62
1.775	11	173	51.43
1.744	4	662	52.42
1.728	4	513	52.96
1.719	3	771	53.25
1.690	6	533	54.25
1.683	8	373	54.49
1.669	7	4 \cdot 10 \cdot 2	54.96
1.653	6	5 \cdot 11 \cdot 1	55.55
1.606	8	2 \cdot 12 \cdot 2,2 \cdot 14 \cdot 0	57.34
1.599	4	004	57.61
1.566	2	931	58.95
1.562	3	880	59.11
1.549	3	224	59.65
1.532	6	573	60.37

Cesium iron chloride hydrate, $\text{Cs}_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation at room temperature of a 2:1 molar aqueous solution of CsCl and FeCl_3 .

Color

Deep reddish orange.

Structure

Orthorhombic, $\text{Amam}(63)$, $Z=4$. Perloff [1976] by single crystal study found that $\text{Cs}_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ was isostructural with $\text{Cs}_2\text{RuCl}_5 \cdot \text{H}_2\text{O}$. The structure of $\text{Cs}_2\text{RuCl}_5 \cdot \text{H}_2\text{O}$ had been determined by Hopkins et al. [1966].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 8.070(1) \text{ \AA} \\ b &= 17.326(2) \\ c &= 7.436(1) \end{aligned}$$

Volume

$$1039.8 \text{ \AA}^3$$

Density

(calculated) 3.302 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 1.9(2)$$

References

Hopkins, T. E., Zalkin, A., Templeton, D. H., and Adamson, M. G. (1966). *Inorg. Chem.* 5, 1431.
Perloff, A. (1976). Private communication.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
d(Å)	I	hkl	2 θ (°)
6.83	8	011	12.95
5.91	7	120	14.97
5.21	4	111	17.00
4.565	40	031	19.43
4.335	6	040	20.47
4.037	45	200	22.00
3.973	100	131	22.36
3.816	5	140	23.29
3.719	25	002	23.91
3.660	4	220	24.30
3.476	12	211	25.61
3.418	3	022	26.05
3.143	10	122,051	28.37
3.024	20	231	29.52
2.950	75	240	30.27

d(Å)	I	hkl	2 θ (°)
2.888	8	060	30.94
2.822	55	042	31.68
2.736	95	202	32.71
2.721	45	160	32.89
2.665	5	142	33.60
2.571	4	320	34.87
2.502	2	311	35.86
2.479	4	251	36.20
2.454	4	013	36.59
2.349	2	071,260+	38.29
2.318	20	331	38.82
2.286	4	340	39.39
2.280	5	062	39.49
2.255	11	171	39.95
2.194	25	162	41.10
2.165	13	080	41.68
2.113	4	322	42.76
2.093	3	180	43.20
2.018	12	400,053	44.89
1.984	12	233	45.70
1.968	4	360	46.08
1.934	2	411	46.94
1.908	4	280	47.62
1.872	4	082	48.60
1.859	11	004	48.97
1.845	6	431	49.36
1.829	3	440	49.82
1.823	3	182	49.99
1.804	4	253	50.56
1.773	8	402,124	51.51
1.770	10	371	51.61
1.739	18	362,333	52.59
1.711	6	173	53.51
1.697	16	282,451	53.98
1.693	12	1·10·0	54.12
1.654	2	460	55.53
1.640	8	442	56.00
1.591	4	2·10·0	57.90
1.587	4	520	58.06
1.573	8	244	58.65
1.570	9	511,0·10·2	58.75
1.535	6	164	60.25
1.533	5	391	60.34
1.5207	6	093	60.87
1.5126	6	540	61.23
1.5101	6	433	61.34
1.4757	4	480	62.93
1.4565	3	3·10·0	63.86
1.4088	6	560	66.29

Copper phosphate, $\text{Cu}(\text{PO}_3)_2$

Sample

The sample was made by heating CuCO_3 and H_3PO_4 together at 760 °C for 45 minutes.

Color

Very pale green

Structure

Monoclinic, I2/a (15) or Ia (9), Z = 8, [Beucher and Grenier, 1968]. Those authors gave the cell in the settings C2/c (15) or Cc (9).

NBS lattice constants of this sample:

$$\begin{aligned} a &= 11.584(2) \text{ \AA} \\ b &= 8.081(2) \\ c &= 9.569(2) \\ \beta &= 107.91(2)^\circ \end{aligned}$$

Volume

$$852.3 \text{ \AA}^3$$

Density

(calculated) 3.452 g/cm³

Reference Intensity

$$I/I_{\text{corundum}} = 1.4$$

Additional patterns

1. PDF card 21-998 [Ball, 1968]
2. PDF card 25-1196 [Smith et al., 1974]

References

- Ball, M. C., (1968). J. Chem. Soc. (London) 5A, 1113.
- Beucher, M., and Grenier, J-C., (1968). Mater. Res. Bull. 3, 643.
- Smith, D. K., et al., Annual Report to the Joint Committee on Powder Diffraction Standards, 1974.

CuK α_1 λ = 1.540598 Å; temp. 25±1 °C			
Internal standard Si, a = 5.43088 Å			
d(Å)	I	hkl	2 θ (°)
6.52	7	110	13.56
6.046	55	011	14.64
5.507	5	200	16.08
4.565	20	211	19.43
4.205	4	202	21.11
4.101	35	112	21.65
3.716	30	211	23.93
3.645	10	121	24.40
3.448	40	112	25.82
3.376	17	121	26.38

d(Å)	I	hkl	2 θ (°)
3.343	50	310	26.64
3.259	10	220	27.34
2.912	100	222	30.68
2.841	30	013	31.46
2.783	8	321	32.14
2.756	35	400	32.46
2.727	12	411	32.82
2.617	2	130	34.23
2.447	25	222	36.69
2.423	6	231	37.08
2.334	17	411	38.55
2.301	8	323	39.11
2.277	7	420,004	39.55
2.190	8	314	41.19
2.127	4	510	42.47
2.101	6	404	43.02
2.089	10	402	43.28
2.049	6	224	44.17
2.030	25	233	44.59
2.007	4	521	45.14
1.877	5	523	48.46
1.861	6	215	48.89
1.835	4	332	49.63
1.821	4	242	50.05
1.779	7	233	51.32
1.738	25	512,334 +	52.61
1.735	16	622	52.73
1.709	6	604	53.59
1.6724	5	620	54.85
1.6663	4	611	55.07
1.6378	6	343	56.11
1.6293	8	440	56.43
1.5906	8	051	57.93
1.5743	6	624	58.59
1.5600	13	235,215	59.18
1.5450	5	710,406	59.81
1.5411	4	116	59.98
1.5385	4	404	60.09
1.5204	9	541,633	60.88
1.5106	12	044	61.32
1.4932	3	435	62.11
1.4876	7	433,152	62.37
1.4827	5	226	62.60
1.4563	9	516,444	63.87

Lead chromium oxide, Pb_2CrO_5

Sample

The sample was prepared by T. Negas by heating PbO (massicot) and Cr_2O_3 together at 630-650 °C for 92 hours followed by regrinding and heating.

Color

Deep orange.

Structure

Monoclinic I2/m (12), $Z = 4$, isostructural with Pb_2SO_5 . The structure has been studied by Ruckman et al. [1972]. These authors gave the cell in a setting in C2/m (12).

NBS lattice constants of this sample:

$$\begin{aligned} a &= 12.728(1) \text{ \AA} \\ b &= 5.6782(5) \\ c &= 7.1414(6) \\ \beta &= 95.23(1)^\circ \end{aligned}$$

Volume

$$513.96 \text{ \AA}^3$$

Density

(calculated) 7.061 g/cm³

Reference Intensity

$$I/I_{\text{corundum}} = 5.1(3)$$

Additional patterns

1. PDF card 26-832 [Ruckman et al., 1972].
2. Negas [1968].

References

Negas, T., (1968). J. Am. Ceram. Soc. 51, 716.
Ruckman, J. C., Morrison, R. T. W., and Buck, R. H. (1972). J. Chem. Soc. Dalton Trans. 1972, 426.

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. 25±1 °C

Internal standard W, $a = 3.16524 \text{ \AA}$

$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
6.46	16	$\bar{1}01$	13.69
6.34	16	200	13.95
5.973	12	101	14.82
5.184	2	110	17.09
4.438	13	011	19.99
3.786	9	$\bar{3}01$	23.48
3.737	4	$\bar{2}11$	23.79
3.555	3	002	25.03
3.542	6	211	25.12
3.390	100	310	26.27
3.230	15	$\bar{2}02$	27.59
3.169	1	400	28.14
2.984	80	202, $\bar{1}12$	29.92
2.881	20	112	31.02
2.838	35	020	31.50
2.651	4	$\bar{4}11$	33.78
2.601	2	$\bar{1}21$	34.46
2.592	4	220	34.58
2.564	6	121	34.96
2.512	15	411	35.72
2.480	16	$\bar{4}02$	36.19
2.460	8	$\bar{5}01$	36.49
2.368	8	$\bar{1}03,312$	37.96
2.314	12	510	38.88
2.272	13	$\bar{3}21$	39.64
2.266	16	402	39.75
2.204	2	321	40.92
2.188	5	013	41.23
2.132	6	$\bar{2}22$	42.36
2.113	10	600	42.77
2.058	20	222	43.97
2.018	2	$\bar{5}12$	44.88
1.992	5	303	45.50
1.951	4	$\bar{6}11$	46.51
1.875	9	$\bar{4}13$	48.50
1.869	19	512, $\bar{4}22$	48.68
1.860	8	$\bar{5}21$	48.94
1.830	2	031	49.80
1.820	2	$\bar{1}23$	50.09
1.7972	1	521	50.76
1.7779	9	004	51.35
1.7708	11	422	51.57
1.7541	5	$\bar{2}04$	52.10
1.7469	1	602,231	52.33
1.7273	11	330	52.97
1.7177	5	701	53.29
1.6947	7	620	54.07
1.6654	11	$\bar{1}32$	55.10
1.6627	4	114	55.20
1.6473	3	132	55.76

Lead chromium oxide, Pb_2CrO_5 - (Continued)

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$
1.6304	5	323	56.39
1.6240	4	$\bar{3}14$	56.63
1.6076	8	$\bar{7}12$	57.26
1.5876	1	$\bar{6}13$	58.05
1.5841	2	800	58.19
1.5753	2	$\bar{6}22$	58.55
1.5682	3	431	58.84
1.5291	10	$\bar{5}23, 314$	60.50
1.5197	8	$\bar{8}11$	60.91
1.5068	9	024, $\bar{7}03$	61.49
1.5020	4	712	61.71
1.4919	4	$\bar{2}24$	62.17
1.4789	2	033	62.78
1.4699	10	$\bar{5}14, 721$	63.21
1.4593	4	613, $\bar{2}33$	63.72
1.4313	2	523	65.12
1.4260	2	$\bar{6}04$	65.39
1.4195	5	040	65.73
1.3991	2	105, $\bar{6}31$	66.81

Lead hydrogen arsenate (schultenite), PbHAsO_4

Sample

The sample was precipitated by adding a concentrated aqueous solution of $\text{Pb}(\text{NO}_3)_2$ to one of As_2O_5 .

Color

Colorless

Optical data

Biaxial (+), $N_\alpha = 1.890$, $N_\beta = 1.910$, $N_\gamma = 1.976$, 2V is medium.

Structure

Monoclinic, $P2/a$ (13), $Z = 2$. [Claringbull, 1950].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 5.8421(6) \text{ \AA} \\ b &= 6.7545(6) \\ c &= 4.8575(6) \\ \beta &= 95.40(1)^\circ \end{aligned}$$

Volume

$$190.83 \text{ \AA}^3$$

Density

(calculated) 6.041 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 7.6(2)$$

Additional patterns

1. PDF card 11-141 [Claringbull, 1950]
2. Hanawalt et al., [1938]

References

Claringbull, G. F., (1950). Mineral. Mag. 29, 287.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
d(Å)	I	hkl	2 θ (°)
6.74	25	010	13.12
4.833	12	001	18.34
4.410	18	110	20.12
3.931	4	011	22.60
3.376	100	$\bar{1}11, 020$	26.38
3.149	70	111	28.32
2.919	13	120	30.60
2.909	25	200	30.71
2.769	6	021	32.30
2.671	5	210	33.52
2.603	4	$\bar{2}01$	34.43
2.555	16	$\bar{1}21$	35.10
2.450	5	121	36.65
2.419	11	002	37.14
2.395	5	201	37.53

d(Å)	I	hkl	2 θ (°)
2.276	1	012	39.56
2.252	6	030	40.00
2.204	16	220	40.92
2.187	7	$\bar{1}12$	41.24
2.100	3	130	43.04
2.061	6	$\bar{2}21$	43.89
2.041	3	031	44.34
1.967	11	022	46.12
1.951	12	$\bar{2}02, \bar{1}31$	46.51
1.9024	6	131	47.77
1.8751	2	$\bar{2}12$	48.51
1.8636	4	310	48.83
1.8203	2	$\bar{1}22$	50.07
1.7939	10	311	50.86
1.7802	14	230	51.28
1.7200	1	212	53.21
1.7029	1	$\bar{2}31$	53.79
1.6886	11	040, 311 +	54.28
1.6820	6	320	54.51
1.6484	5	032	55.72
1.6410	2	231	55.99
1.6298	3	321	56.41
1.6217	2	140	56.72
1.6123	2	$\bar{1}32, 003$	57.08
1.5939	< 1	041	57.80
1.5740	5	222	58.60
1.5590	3	132	59.22
1.5497	10	$\bar{1}41, 321 +$	59.61
1.5254	5	141	60.66
1.4806	5	113	62.70
1.4749	5	$\bar{2}32$	62.97
1.4606	2	240	63.66
1.4542	3	023, 400	63.97
1.4404	2	$\bar{1}23$	64.66
1.4346	2	331	64.95
1.4157	1	312	65.93
1.3954	2	232	67.01
1.3842	2	042, 123	67.63
1.3788	2	331	67.93
1.3634	< 1	$\bar{1}42$	68.80
1.3507	2	050	69.54
1.3353	2	420	70.46
1.3167	1	$\bar{4}21$	71.61
1.3102	< 1	033	72.02
1.3010	3	$\bar{4}02, 051$	72.61
1.2774	3	$\bar{4}12, \bar{3}13 +$	74.17
1.2592	1	$\bar{4}21, 223$	75.43
1.2503	2	$\bar{3}41$	76.06
1.2251	3	250, 242	77.92
1.2132	4	341	78.83
1.1990	2	$\bar{2}51$	79.95
1.1972	1	402	80.09
1.1791	2	052, 412	81.58
1.1766	2	251	81.79
1.1679	2	313	82.53
1.1586	2	$\bar{1}43$	83.34
1.1564	2	342	83.54

Lithium silicate, Li_2SiO_3

Sample

The sample was prepared by heating a 1:1 molar mixture of Li_2CO_3 and dried silica gel at 860 °C for 5 minutes; the material was ground and reheated for 5 minutes at 860 °C. A final heating for several minutes at about 1200 °C followed.

Color

Colorless

Structure

Orthorhombic, $\text{Ccm}2_1(36)$, $Z = 4$, [Seeman, 1956], isostructural with Na_2SiO_3 , low $(\text{Na,Li})\text{SiO}_3$ [West, 1976] and Li_2GeO_3 [Völlenklee and Wittman, 1968].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 5.3975(6) \text{ \AA} \\ b &= 9.3974(6) \\ c &= 4.6615(5) \end{aligned}$$

Volume

$$236.44 \text{ \AA}^3$$

Density

(calculated) 2.527 g/cm³

Additional patterns

1. PDF card 15-519 [Lam, Sheffield, England].
2. West [1976].

References

- Seemann, H. (1956). Acta Crystallogr. 9, 251.
Völlenklee, H., and Wittmann, A. (1968). Monatsh. Chem. 99, 244.
West, A. R. (1976). J. Am. Ceram. Soc. 59, 118.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. 25 \pm 1 °C			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
d (Å)	I	hkl	2 θ (°)
4.69	100	020,110	18.91
3.301	65	111	26.99
2.708	65	130	33.05
2.700	45	200	33.15
2.342	19	131,220	38.41
2.331	20	002	38.60
2.091	7	221	43.24
2.085	5	022,112	43.36
1.7747	4	150	51.45
1.7667	9	310,132	51.70
1.7638	8	202	51.79
1.6563	7	241	55.43
1.6522	7	311,222	55.58
1.5665	12	060	58.91
1.5605	15	330	59.16
1.4747	3	113	62.98
1.4105	1	242	66.20
1.4079	1	312	66.34
1.3547	3	260	69.31
1.3475	5	133	69.73
1.3001	5	062,350	72.67
1.2965	8	332,401 +	72.90
1.2544	3	171	75.77
1.2495	2	421	76.12
1.1747	2	080	81.95
1.1710	2	262	82.27
1.1681	2	243,402	82.52
1.1350	3	352,441	85.48
1.0770	<1	280	91.32
1.0759	<1	370	91.44
1.0700	<1	204	92.09
1.0488	1	082	94.52
1.0452	1	511	94.95
1.0441	<1	044	95.08
1.0253	1	190	97.40
1.0212	2	263	97.93
1.0188	1	403	98.24
1.0013	1	191	100.58
0.9984	2	461,173	100.98
0.9778	<1	282	103.96
0.9769	<1	372	104.10
0.9738	1	244	104.57
0.9727	<1	314	104.73
0.9397	<1	0 \cdot 10 \cdot 0	110.12
0.9384	<1	192	110.34
0.9348	1	532,443 +	110.98
0.9337	1	334	111.18

Lithium tantalum oxide, LiTaO_3

Sample

The sample was prepared as a precipitate by adding LiOH to a solution of hydrolyzed Ta_2O_5 . This was further crystallized by heating at 860°C overnight.

Color

Colorless

Structure

Hexagonal, $R3c$ (161), $Z=6$, by analogy with LiNbO_3 which was studied by Bailey [1952].

NBS lattice constants of this sample:

$$a = 5.1530(4) \text{ \AA}$$

$$c = 13.755(2)$$

Volume

$$316.30 \text{ \AA}^3$$

Reference intensity

$$I/I_{\text{corundum}} = 11.8(5)$$

Density

(calculated) 7.430 g/cm^3

Additional pattern

1. PDF card 9-187 [Lapickij and Simanov, 1955].

References

Bailey, P., thesis, Bristol (1952) quoted by Megaw, H. D. (1954). *Acta Cryst.* **7**, 187.
Lapickij, A. V. and Simanov, J. P. (1955). *Zh. Fiz. Khim.* **29**, 1201.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ\text{C}$			
Internal standard Si, $a = 5.43088 \text{ \AA}$			
$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
3.745	100	012	23.74
2.723	40	104	32.86
2.577	25	110	34.79
2.292	4	006	39.28
2.245	3	113	40.13
2.122	14	202	42.57
1.871	16	024	48.62
1.712	20	116	53.48
1.638	14	122	56.12
1.604	6	018	57.41
1.5139	11	214	61.17
1.4874	6	300	62.38
1.3621	3	208	68.88
1.3145	3	119, $1 \cdot 0 \cdot 10$	71.75
1.2883	3	220	73.44
1.2481	3	306	76.22
1.2183	4	312	78.44
1.2043	4	128	79.53
1.1710	2	$0 \cdot 2 \cdot 10$	82.27
1.1648	4	134	82.80
1.1463	1	$0 \cdot 0 \cdot 12$	84.44
1.1231	3	226	86.61
1.10.2	1	042	88.78
1.0664	2	$2 \cdot 1 \cdot 10$	92.50
1.0471	2	$137, 1 \cdot 1 \cdot 12$	94.72
1.0126	2	232	99.06
1.0047	2	$318, 1 \cdot 2 \cdot 11$	100.12
0.9812	2	324	103.45
.9740	2	410	104.54

Manganese phosphate, $\text{Mn}(\text{PO}_3)_2$

Sample

The sample was prepared by melting MnCl_2 with H_3PO_4 in molar proportions of 1:2.

Color

Pale pink

Structure

Monoclinic, $I2/a$ (15) or Ia (9), $Z = 8$ [Beucher and Grenier, 1968]. Those authors gave the cell in the settings $C2/c$ (15) or Cc (9).

NBS lattice constants of this sample

$$\begin{aligned} a &= 11.359(2) \text{ \AA} \\ b &= 8.472(2) \\ c &= 10.176(2) \\ \beta &= 112.06^\circ(2) \end{aligned}$$

Volume

$$907.57 \text{ \AA}^3$$

Density

(calculated) 3.116 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 0.89(11)$$

Additional pattern

1. PDF card 21-554 [Lee and Browne, 1968].

References

Beucher, M., and Grenier, J. C., (1968). Mater. Res. Bull. 3, 643.

Lee, J. D., and Browne, L. S., (1968). J. Chem. Soc. A 559.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$			
Internal standard Si, $a = 5.43088 \text{ \AA}$			
$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
6.29	30	011	14.06
5.26	4	200	16.85
4.71	13	002	18.81
4.65	13	$\bar{2}11$	19.07
4.348	35	$\bar{1}12$	20.41
3.613	20	211	24.62
3.468	30	112	25.67
3.300	10	220	27.00
3.242	35	$\bar{3}10$	27.49
3.065	100	$\bar{2}22$	29.11
2.998	3	202	29.78
2.947	20	013	30.30
2.728	3	$\bar{1}30$	32.80
2.681	4	$\bar{4}11$	33.39
2.632	20	400	34.03
2.521	5	$\bar{2}31$	35.59
2.446	20	222	36.71
2.424	7	$\bar{3}23$	37.06
2.358	3	004	38.13
2.331	9	$\bar{3}14, \bar{4}22$	38.59
2.236	11	$411, 420$	40.30
2.218	2	404	40.64
2.200	2	330	41.00
2.175	4	$\bar{2}24$	41.48
2.145	19	$\bar{2}33$	42.09
2.118	4	040	42.66
2.001	6	402	45.29
1.979	5	$\bar{2}15$	45.81
1.965	2	$\bar{4}24, 240$	46.16
1.928	3	$\bar{5}23$	47.11
1.890	3	$\bar{4}33$	48.10
1.864	4	$\bar{4}15$	48.82
1.839	6	$\bar{3}34$	49.54
1.802	7	$\bar{1}25, \bar{2}33$	50.60
1.767	5	$\bar{5}32$	51.70
1.735	4	224	52.71
1.728	11	$242, \bar{6}22$	52.93
1.687	2	$\bar{4}42$	54.35
1.667	10	051, $\bar{5}12$	55.05
1.6503	12	440, $\bar{4}06$	55.65

Nickel phosphate, $\text{Ni}(\text{PO}_3)_2$

Sample

The sample was prepared by heating a 1:2 molar mixture of NiCO_3 and H_3PO_4 at about 700°C for 15 hours. It was reground and heated to 1000°C for 15 hours.

Color

Light yellowish green

Structure

Monoclinic, $\text{I2/a}(15)$ or $\text{Ia}(9)$, $Z=8$, [Beucher and Grenier, 1968]. These authors gave the cell in the settings $\text{C2/c}(15)$ or $\text{Cc}(9)$.

NBS lattice constants of this sample:

$$\begin{aligned} a &= 11.086(3)\text{\AA} \\ b &= 8.227(2) \\ c &= 9.832(3) \\ \beta &= 112.74(3)^\circ \end{aligned}$$

Volume

$$826.9 \text{ \AA}^3$$

Density

(calculated) 3.480 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 1.7$$

Additional pattern

1. PDF card 19-835 (Sarver, 1966).

References

Beucher, M. and Grenier, J. C. (1968). Mater. Res. Bull. 3, 643.
Sarver, J. F. (1966). Trans. Brit. Ceram. Soc. 65, 191.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ\text{C}$			
Internal standard W, $a = 3.16524 \text{ \AA}$			
$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
6.39	7	110	13.84
6.08	50	011	14.55
5.11	3	200	17.33
4.53	20	$\bar{2}11$	19.56
4.321	3	$\bar{2}02$	20.54
4.209	40	$\bar{1}12$	21.09
3.711	5	$\bar{1}21$	23.96
3.493	19	211	25.48
3.339	30	112	26.68
3.205	11	220	27.81
3.148	30	310	28.33
3.049	4	022	29.27
2.979	100	$\bar{2}22$	29.97
2.836	25	013	31.52
2.748	2	$\bar{3}21$	32.56
2.650	2	$\bar{1}30$	33.80
2.612	4	$\bar{4}11$	34.31
2.557	25	$400, \bar{1}23$	35.06
2.451	4	$\bar{2}31$	36.64
2.359	25	$\bar{3}23$	38.11
2.263	8	$\bar{3}14$	39.81
2.220	2	123	40.60
2.165	13	$\bar{4}11$	41.69
2.135	3	$330, \bar{5}12$	42.29
2.106	3	$\bar{2}24$	42.90
2.081	20	$\bar{2}33$	43.44
2.057	4	040	43.99
2.001	2	$\bar{1}41$	45.28
1.936	4	141	46.90
1.929	7	$402, \bar{5}21$	47.07
1.912	5	$\bar{2}15$	47.52
1.882	2	$\bar{5}23$	48.33
1.856	2	$\bar{2}42$	49.03
1.848	2	$\bar{6}02$	49.26
1.8102	3	$\bar{4}15$	50.37
1.7968	3	$\bar{3}41$	50.77
1.7857	4	$\bar{3}34$	51.11
1.7638	2	$\bar{6}11$	51.79
1.7392	9	$\bar{1}43, 233 +$	52.58
1.7215	5	$\bar{5}32$	53.16
1.6858	7	$\bar{6}22, 521$	54.38
1.6740	3	$\bar{3}43, 242$	54.79
1.6704	3	224	54.92
1.6193	7	051	56.81
1.5976	10	$\bar{2}35$	57.65
1.5759	1	$\bar{2}44, \bar{2}51$	58.52
1.5577	2	$\bar{1}16$	59.27
1.5534	4	125	59.45
1.5233	7	044	60.74

Potassium barium chromium oxide, $K_2Ba(CrO_4)_2$

Sample

The sample was prepared by heating $K_2Cr_2O_7$ and $BaCO_3$ in a 1:1 molar ratio at 750 °C for 1 hour followed by grinding and heating for 18 hours at 750 °C.

Color

Light greenish yellow

Structure

Hexagonal, $R\bar{3}m(166)$. $Z = 3$, isostructural with $Sr_3(PO_4)_2$ and many double sulfates and chromates [Schwarz, 1966]. The structure of $Sr_3(PO_4)_2$ was determined by Wilhelmi [1967] and $(NH_4)_2Pb(SO_4)_2$ was determined by Møller [1954].

NBS lattice constants of this sample:

$$a = 5.7292(5) \text{ \AA}$$

$$c = 21.512(3)$$

Volume

$$611.51 \text{ \AA}^3$$

Density

(calculated) 3.645 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 3.3(2)$$

Additional pattern

1. PDF card 19-937 [Schwarz, 1966].

References

Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344, 41.
Wilhelmi, K.-A., (1967). Ark. Kemi 26, 157.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. 25 \pm 1 °C			
Internal standard Si, $a = 5.43088 \text{ \AA}$			
d (Å)	I	hkl	2 θ (°)
7.16	15	003	12.36
4.83	4	101	18.36
4.503	30	012	19.70
3.642	3	104	24.42
3.590	2	006	24.78
3.251	100	015	27.41
2.864	70	110	31.21
2.661	14	113	33.65
2.612	8	107	34.31
2.464	2	021	36.43
2.416	3	202	37.18
2.390	7	009	37.61
2.252	11	024	40.00
2.238	8	116	40.26
2.149	30	205	42.01
1.973	20	1•0•10	45.95
1.868	2	211	48.70
1.848	4	122	49.27
1.836	5	119	49.60
1.8234	3	208	49.98
1.7926	3	0•0•12	50.90
1.7188	15	125	53.25
1.6538	9	300	55.52
1.6253	7	0•2•10	56.58
1.6118	3	303	57.10
1.6007	2	217	57.53
1.5200	3	1•1•12	60.90
1.5017	2	306	61.72
1.4676	2	0•1•14	63.32
1.4321	9	220	65.08
1.4134	10	2•1•10	66.05
1.4045	1	223	66.52
1.3766	2	0•2•13	68.05
1.3731	1	131	68.25
1.3650	2	312	68.71
1.3600	2	309	69.00
1.3533	1	1•2•11	69.39
1.3108	5	315	71.98
1.2823	7	1•1•15	73.84
1.2561	1	137	75.65
1.2289	2	229	77.63
1.2260	1	0•1•17	77.85
1.2157	2	3•0•12	78.64

Potassium barium molybdenum oxide, $K_2Ba(MoO_4)_2$

Sample

The sample was made by melting together MoO_3 , K_2CO_3 and $BaCO_3$ in a molar ratio of 2:1:1, followed by grinding and reheating.

Color

Colorless

Structure

Hexagonal, $R\bar{3}m(166)$, $Z = 3$, isostructural with $K_2Pb(SO_4)_2$, $Sr_3(PO_4)_2$ and other double chromates and sulfates [Trunin et al., 1975]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Möller [1954].

NBS lattice constants of this sample:

$$a = 6.0051(4) \text{ \AA}$$

$$c = 21.324(2)$$

Volume

$$665.96 \text{ \AA}^3$$

Density

(calculated) 4.004 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 4.2(3)$$

Additional pattern

1. Trunin et al. [1975].

References

Möller, C. K., (1954). Acta Chem. Scand. 8, 81.
Trunin, A. S., Shter, G. E., and Serezhkin, V. N., (1975). Russ. J. Inorg. Chem. 20, 1227.

$CuK\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$

Internal standard W, $a = 3.16524 \text{ \AA}$

$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
7.104	9	003	12.45
5.055	7	101	17.53
4.677	20	012	18.96
3.719	4	104	23.91
3.552	3	006	25.05
3.296	100	015	27.03
3.001	90	110	29.75
2.765	8	113	32.35
2.629	7	107	34.08
2.370	1	009	37.94
2.338	2	024	38.48
2.220	35	205	40.61
1.973	25	10010	45.97
1.933	2	122	46.96
1.861	2	208,119	48.90
1.844	2	214	49.37
1.785	20	125	51.12
1.734	11	300	52.76
1.684	2	303	54.43
1.649	9	02010	55.70
1.530	3	11012	60.46
1.5009	8	220	61.76
1.4450	10	21010	64.43
1.4295	2	312	65.21
1.4214	2	00015	65.63
1.3664	6	315	68.63
1.3036	2	137	72.44
1.2852	7	11015	73.65
1.2438	4	045	76.53
1.1945	4	13010	80.31
1.1860	2	02016,232	81.01
1.1491	4	235	84.19
1.1351	4	410	85.47
1.1206	2	413	86.85
1.1106	3	327	87.83
1.0993	4	30015	88.97
1.0445	2	01020	95.04
1.0323	2	22015	96.52

Potassium calcium sulfate hydrate (syngenite), $K_2Ca(SO_4)_2 \cdot H_2O$

Sample

The sample was prepared by mixing equal volumes of saturated aqueous solutions of $CaSO_4$ and K_2SO_4 , and evaporating slowly at room temperature. The first crystals formed were used. The crystals were acicular.

Color

Colorless

Optical data

$n_\alpha = 1.500$, $n_\gamma = 1.518$ [Aruja, 1958].

Structure

Monoclinic, $P2_1/m$ (11), $Z=2$ [Laszkiewicz, 1936]
The structure of $K_2Ca(SO_4)_2 \cdot H_2O$ has been refined by Corazza and Sabelli [1967] and by Gorogotskaya et al. [1968].

NBS lattice constants of this sample

$$\begin{aligned} a &= 9.777(2) \text{ \AA} \\ b &= 7.147(2) \\ c &= 6.250(2) \\ \beta &= 104.01(2)^\circ \end{aligned}$$

Volume

$$423.7 \text{ \AA}^3$$

Density

(calculated) 2.574 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 1.05(6)$$

Additional patterns

1. PDF card 11-117 [Aruja, 1958],
2. Baynham and Raistrick [1960].

References

- Aruja, E. (1958). Mineral Mag. 31, 943.
Baynham, J. W. and Raistrick, B. (1960). In Chemistry and Technology of Fertilizers (Reinhold, N. Y.). ACS Monogr. Ser. 148, Chap. 21, p. 358.
Corazza, E. and Sabelli, K. (1967). Z. Krist. 124, 398.
Gorogotskaya, L. I., Podberezskaya, N. V. and Borisov, S. V. (1968). Zh. Strukt. Khim., SSSR, 9 #1, 86.
Laszkiewicz, A. (1936). Arch. Mineral. 12, 8.

$CuK\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$

Internal standard W, $a = 3.16524 \text{ \AA}$

$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
9.49	40	100	9.31
5.71	55	110	15.51
4.74	16	200	18.71
4.624	40	011	19.18
4.496	30	111	19.73
3.954	20	210	22.47
3.887	30	111	22.86
3.572	30	020	24.91
3.347	35	120	26.61
3.165	75	300	28.17
3.114	17	$\bar{3}01, \bar{1}02$	28.64
3.036	35	002	29.40
2.891	30	$\bar{2}02, 310$	30.91
2.855	100	$\bar{1}12, 220$	31.31
2.827	50	121	31.62
2.791	20	012	32.04
2.741	55	$\bar{2}21$	32.64
2.704	15	102	33.10
2.560	2	301	35.02
2.513	30	$\bar{3}02$	35.70
2.447	7	221	36.69
2.411	8	311	37.26
2.371	20	$400, \bar{3}12$	37.91
2.355	25	$\bar{3}21$	38.18
2.312	16	$022, 130$	38.93
2.288	7	$\bar{4}11$	39.34
2.250	4	$410, \bar{2}22$	40.04
2.129	5	230	42.42
2.081	14	$321, \bar{2}31$	43.46
2.046	17	$\bar{2}03, \bar{4}12$	44.23
2.002	9	$\bar{4}21$	45.27
1.974	8	420	45.90
1.965	25	302	46.15
1.9498	20	$\bar{5}01$	46.54
1.9447	20	$013, 231$	46.67
1.9028	12	330	47.76
1.8968	13	$500, \bar{3}31$	47.92
1.8924	12	$\bar{1}32$	48.04
1.8333	6	$510, \bar{4}22$	49.69
1.7870	20	$132, 040$	51.07
1.7763	7	$421, \bar{2}23$	51.40
1.7444	4	331	52.41
1.6755	7	520	54.74
1.6293	2	601	56.43
1.5812	6	$\bar{4}23, 600$	58.31
1.5559	11	340	59.35
1.5436	5	610	59.87
1.5293	7	$\bar{6}12$	60.49
1.4781	4	133	62.82
1.4518	8	$\bar{5}23$	64.09

Potassium calcium sulfate hydrate (syngenite), $K_2Ca(SO_4)_2 \cdot H_2O$ - (continued)

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$
1.4466	6	601, $\bar{4}$ 04	64.35
1.4278	5	$\bar{2}$ 24, $\bar{1}$ 24 +	65.30
1.3964	3	$\bar{7}$ 01, $\bar{6}$ 13	66.96
1.3701	4	$\bar{4}$ 42	68.42
1.3494	6	522	69.62
1.3413	4	621	70.10
1.3314	4	710, $\bar{5}$ 14	70.70
1.3217	8	342, $\bar{5}$ 33	71.30
1.3085	5	$\bar{3}$ 43	72.13
1.2803	5	$\bar{3}$ 34	73.98
1.2669	3	$\bar{5}$ 24	74.89

Potassium iron chloride hydrate (erythrosiderite), $K_2FeCl_5 \cdot H_2O$

Sample

The sample was made by slow evaporation at room temperature of an acid solution of KCl and $FeCl_3$.

Optical Data

Biaxial (+), $N_\alpha = 1.712$, $N_\beta = 1.75$, $N_\gamma = 1.795$
2V is medium large.

Color

Deep reddish orange

Structure

Orthorhombic, Pmnb (62), Z=4, isostructural with $(NH_4)_2FeCl_5 \cdot H_2O$. The structure was determined by Bellanca [1947].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 9.706(3) \text{ \AA} \\ b &= 13.585(3) \\ c &= 7.018(1) \end{aligned}$$

Volume

925.3 \AA^3

Density

(calculated) 2.364 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 1.9$

Additional patterns

1. PDF card 25-1160, natural mineral [Mandarino, Toronto, Ontario].

Reference

Bellanca, A. (1947). Ric. Sci. Ricostr. 17, 1360.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. 25 \pm 1 $^\circ\text{C}$			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
5.68	35	101	15.59
5.566	40	120	15.91
5.248	4	111	16.88
4.878	14	021	18.17
3.832	2	211	23.19
3.541	2	131	25.13
3.507	2	002	25.38
3.440	10	221	25.88
3.397	12	012,040	26.21
3.208	2	112,140	27.79
3.056	14	041	29.20
2.993	19	231	29.83
2.969	5	122	30.07
2.934	8	301	30.44
2.920	10	320	30.59
2.841	16	202	31.46
2.782	100	212,240	32.15
2.589	3	241	34.62
2.440	25	042	36.81
2.427	40	400	37.01
2.365	2	142	38.02
2.306	2	013	39.02
2.244	3	322,113	40.16
2.211	4	023	40.77
2.180	5	242	41.39
2.149	12	052	42.00
2.099	6	152	43.07
2.078	4	033	43.51
2.032	8	133	44.55
1.995	2	351	45.43
1.970	6	261	46.04
1.911	3	233	47.54
1.902	6	062,441	47.79
1.890	3	143	48.10
1.872	8	501,071	48.61
1.868	6	162,520	48.72
1.826	12	432,323	49.91
1.789	4	352	51.01
1.7711	3	262	51.56
1.7484	3	333	52.28
1.7404	5	014	52.54
1.7209	10	442	53.18
1.7123	4	114	53.47
1.6982	6	072,080	53.95
1.6730	4	172,180 +	54.83
1.6560	2	460,343	55.44
1.6500	4	081,204	55.66
1.6392	3	541	56.06
1.6349	5	034,423	56.22
1.6084	8	452	57.23
1.5621	3	281	59.09

Potassium lead chromium oxide, $K_2Pb(CrO_4)_2$

Sample

The sample was prepared by melting a 1:1 molar mixture of K_2CrO_4 and $PbCrO_4$.

Color

Strong yellow

Structure

Hexagonal, $R\bar{3}m$ (166), $Z = 3$, isostructural with Sr_3PO_4 and many double chromates, sulfates and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was determined by Møller [1954].

NBS lattice constants of this sample:

$$a = 5.7173(7) \text{ \AA}$$

$$c = 21.031(3)$$

Volume

$$595.35 \text{ \AA}^3$$

Density

(calculated) 4.329 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 3.8(2)$$

Additional pattern

1. PDF card 19-971 [Schwarz, 1966]

References

Møller, C. K. (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 345, 230.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard Si, $a = 5.43088 \text{ \AA}$			
$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
6.99	30	003	12.65
4.82	19	101	18.39
4.47	40	012	19.83
3.604	8	104	24.68
3.505	2	006	25.39
3.204	100	015	27.82
2.859	85	110	31.26
2.647	20	113	33.84
2.571	8	107	34.87
2.457	4	021	36.54
2.336	6	009	38.50
2.240	11	024	40.23
2.216	11	116	40.69
2.133	30	205	42.34
1.935	19	10010	46.92
1.863	4	211	48.83
1.842	5	122	49.45
1.809	5	119	50.41
1.802	5	208	50.62
1.764	2	214	51.80
1.753	2	00012	52.13
1.7102	19	125	53.54
1.6508	9	300	55.63
1.6066	7	303	57.30
1.6033	7	00210	57.43
1.5884	3	217	58.02
1.4935	3	10112,306	62.10
1.4380	2	00114	64.78
1.4293	7	220	65.22
1.3978	10	20110	66.88
1.3621	2	312	68.88
1.3053	6	315	72.33
1.2586	6	10115	75.47

Potassium lead molybdenum oxide, $K_2Pb(MoO_4)_2$

Sample

The sample was prepared by melting together K_2CO_3 , $PbCO_3$ and MoO_3 , at about 850 °C.

Color

Yellowish white

Structure

Hexagonal, $R\bar{3}m$ (166), $Z = 3$. The similarity of the cell size, powder patterns, and chemistry of $K_2Pb(MoO_4)_2$, $Sr_3(PO_4)_2$, $K_2Pb(SO_4)_2$ (palmierite), and $(NH_4)_2Pb(SO_4)_2$ strongly suggests an isostructural relationship. The structure of $(NH_4)_2Pb(SO_4)_2$ has been studied by Møller [1954].

NBS lattice constants of this sample:

$$a = 5.9853(2) \text{ \AA}$$

$$c = 20.987(1) \text{ \AA}$$

Polymorphism

Belyaev [1961] reports a polymorphic transformation of $K_2Pb(MoO_4)_2$ at 765 °C. No evidence of this was seen in the present work.

Volume

$$651.09 \text{ \AA}^3$$

Density

(calculated) 4.631 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 4.0(3)$$

References

Belyaev, I.N. (1961). Russ. J. Inorg. Chem. 6, 602.
Møller, C. K. (1954). Acta Chem. Scand. 8, 81.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. 25 \pm 1 °C			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
d (Å)	I	hkl	2 θ (°)
6.99	25	003	12.66
4.648	40	012	19.08
3.687	2	104	24.12
3.262	100	015	27.32
2.993	85	110	29.83
2.752	18	113	32.51
2.595	8	107	34.54
2.332	3	009	38.57
2.325	3	024	38.70
2.274	3	116	39.60
2.205	30	205	40.89
1.960	4	027	46.28
1.945	18	1•0•10	46.65
1.925	7	122	47.17
1.843	3	208	49.41
1.7750	25	125	51.44
1.7485	3	0•0•12	52.28
1.7279	12	300	52.95
1.6775	3	303	54.67
1.6397	4	217	56.04
1.6312	7	0•2•10	56.36
1.5694	2	128	58.79
1.5099	3	1•1•12	61.35
1.4961	8	220	61.98
1.4632	2	223	63.53
1.4398	5	0•1•14	64.69
1.4319	9	2•1•10	65.09
1.4245	4	312	65.47
1.3991	2	0•0•15	66.81
1.3602	8	315	68.99
1.2961	2	137	72.93
1.2675	4	1•1•15	74.85
1.2382	3	045	76.94
1.2292	1	3•0•12	77.61
1.2010	1	0•1•17	79.79
1.1860	5	1•3•10	81.01
1.1619	1	048	83.05
1.1442	5	235	84.63
1.1368	3	2•2•12	85.31
1.1312	3	410	85.84
1.1166	1	413	87.24
1.1054	2	327	88.35
1.1028	3	4•0•10	88.61
1.0874	2	3•0•15	90.21

Potassium lead sulfate (palmierite), $K_2Pb(SO_4)_2$

Sample

The sample was prepared by melting a 1:1 molar mixture of K_2SO_4 and $PbSO_4$, grinding and reheating at 450 °C overnight.

Color

Colorless

Structure

Hexagonal, $R\bar{3}m$ (166), $Z = 3$, isostructural with $Sr_3(PO_4)_2$ and many double chromates, sulfates and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample

$$a = 5.4950(6) \text{ \AA}$$

$$c = 20.849(4)$$

Volume

$$545.18 \text{ \AA}^3$$

Density

(calculated) 4.363 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 2.77(10)$$

Additional pattern

1. PDF card 20-902 [Schwarz, 1966]

References

Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344, 41.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. 25 \pm 1 °C			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
d(Å)	I	hkl	2 θ (°)
6.948	35	003	12.73
4.641	25	101	19.11
4.333	45	012	20.48
3.515	18	104	25.32
3.477	3	006	25.60
3.138	100	015	28.42
2.749	70	110	32.54
2.557	35	113	35.07
2.526	13	107	35.51
2.366	9	021	38.00
2.318	10	202,009	38.82
2.287	3	018	39.36
2.166	25	024	41.67
2.156	30	116	41.86
2.068	35	205	43.74
1.910	25	1•0•10	47.57
1.860	2	027	48.94
1.792	10	211	50.92
1.772	20	122,119	51.54
1.760	7	0•1•11	51.92
1.7575	8	208	51.99
1.7373	4	0•0•12	52.64
1.7002	3	214	53.88
1.6516	20	125	55.60
1.5861	11	300	58.11
1.5684	8	0•2•10	58.83
1.5464	5	303	59.75
1.5397	4	217	60.04
1.5195	2	1•0•13	60.92
1.4823	3	2•0•11	62.62
1.4802	3	128	62.72
1.4686	5	1•1•12	63.27
1.4428	6	306	64.54
1.4212	3	0•1•14	65.64
1.3900	2	0•0•15	67.31
1.3734	10	220	68.23
1.3617	14	2•1•10	68.90
1.3479	2	223	69.71
1.3296	2	0•2•13	70.81
1.3169	1	131	71.60
1.3088	3	312,309	72.11
1.3046	3	1•2•11	72.38
1.2792	2	134	74.05
1.2622	<1	2•0•14	75.22
1.2582	9	315	75.50
1.2403	13	1•1•15	76.79
1.2067	2	137	79.34
1.1974	2	2•1•13	80.08
1.1878	2	401,0•1•17	80.86
1.1820	3	042	81.34

Potassium strontium sulfate (kalistrontite), $K_2Sr(SO_4)_2$

Sample

Two and one-half grams of $SrCl_2 \cdot 6H_2O$ in 10 mL H_2O was added dropwise to 20 g K_2SO_4 in 100 mL H_2O at the boiling point and refluxed with stirring for 4 days. The precipitate was filtered at the boiling point, squeezed on blotting paper and dried in dessicator. The crystallinity was improved by heating the precipitate to 600 °C for 3 days.

Color

Colorless

Structure

Hexagonal, $R\bar{3}m(166)$, $Z = 3$, isostructural with $Sr_3(PO_4)_2$ and many double chromates, sulfates, and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

$$a = 5.4630(3) \text{ \AA}$$

$$c = 20.843(1) \text{ \AA}$$

Volume

$$538.73 \text{ \AA}^3$$

Density

(calculated) 3.310 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 3.3(2)$$

Additional patterns

1. PDF card 15-123 Voronova [1962].
2. PDF card 19-996 Schwarz [1966].

References

- Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
 Schwarz, H., (1966). Z. Anorg. Allg. Chem. 344, 41.
 Voronova, M. L., (1962). Zap. Vses. Mineral. Obshchest. 91, 712.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. 25 \pm 1 °C			
Internal standard W, $a = 3.16524 \text{ \AA}$			
d(Å)	I	hkl	2 θ (°)
6.94	15	003	12.75
4.617	1	101	19.21
4.308	17	012	20.60
3.472	1	006	25.64
3.128	100	015	28.51
2.731	65	110	32.77
2.543	11	113	35.27
2.520	4	107	35.60
2.352	2	021	38.24
2.316	8	009	38.85

d(Å)	I	hkl	2 θ (°)
2.308	6	202	39.00
2.153	17	024	41.92
2.148	19	116	42.03
2.0576	25	205	43.97
1.9077	18	1•0•10	47.63
1.7818	3	211	51.23
1.7664	5	119	51.71
1.7622	2	122	51.84
1.7516	3	208	52.18
1.7364	3	0•0•12	52.67
1.6915	<1	214	54.18
1.6435	12	125	55.90
1.5772	7	300	58.47
1.5641	5	0•2•10	59.01
1.5376	2	303	60.13
1.4657	1	1•1•12	63.41
1.4358	2	306	64.89
1.4201	1	0•1•14	65.70
1.3892	2	0•0•15	67.35
1.3655	8	220	68.68
1.3570	9	2•1•10	69.17
1.3400	1	223	70.18
1.3273	1	0•2•13	70.95
1.3033	1	309	72.46
1.3007	2	1•2•11	72.63
1.2723	<1	134	74.52
1.2513	5	315	75.99
1.2384	8	1•1•15	76.93
1.2008	<1	137	79.81
1.1765	1	229	81.80
1.1677	<1	3•0•12	82.55
1.1533	<1	404	83.81
1.1441	1	1•2•14	84.64
1.1410	1	0•2•16	84.93
1.1379	2	045	85.21
1.1105	3	1•3•10	87.84
1.0737	1	2•2•12	91.68
1.0661	1	1•1•18	92.53
1.0506	3	235	94.31
1.0426	4	3•0•15	95.26
1.0324	2	410	96.51
1.0287	1	4•0•10	96.97
1.0210	1	413	97.97
1.0180	1	0•1•20	98.35

Rubidium barium chromium oxide, $\text{Rb}_2\text{Ba}(\text{CrO}_4)_2$

Sample

The sample was prepared by heating a 1:1 molar mixture of $\text{Rb}_2\text{Cr}_2\text{O}_7$ and BaCO_3 together at 750° for 1 hour. This was followed by grinding, and reheating at 750° for 48 hours.

Color

Light greenish yellow

Structure

Hexagonal, $R\bar{3}m(166)$, $Z = 3$, isostructural with $\text{Sr}_3(\text{PO}_4)_2$ and many double sulfates, chromates, and selenates [Schwarz, 1966]. The structure of $(\text{NH}_4)_2\text{Pb}(\text{SO}_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

$$a = 5.8107(6) \text{ \AA}$$

$$c = 22.210(3)$$

Volume

$$649.4 \text{ \AA}^3$$

Density

(calculated) 4.144 g/cm^3

Reference Intensity

$$I/I_{\text{corundum}} = 5.8(2)$$

Additional pattern

1. PDF card 19-1066 [Schwarz, 1966].

References

Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 344, 41.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1^\circ \text{C}$			
Internal standard Si, $a = 5.43088 \text{ \AA}$			
$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
7.39	2	003	11.96
4.90	6	101	18.09
4.58	4	012	19.38
3.731	4	104	23.83
3.326	100	015	26.78
2.905	65	110	30.75
2.705	2	113	33.09
2.683	2	107	33.37
2.500	2	021	35.89
2.467	5	009	36.39
2.455	4	202	36.58
2.430	2	018	36.97
2.291	9	024	39.29
2.287	12	116	39.37
2.189	25	205	41.21
2.031	20	1•0•10	44.57
1.972	1	027	45.99
1.895	2	211	47.96
1.881	5	119	48.34
1.876	3	122	48.49
1.850	1	0•0•12	49.20
1.799	1	214	50.70
1.748	15	125	52.28
1.677	7	300	54.68
1.665	8	0•2•10	55.10
1.528	1	306	60.56
1.513	1	0•1•14	61.19
1.480	2	0•0•15	62.71
1.453	7	220	64.02
1.4448	10	2•1•10	64.44
1.3869	1	309	67.48
1.3314	5	315	70.70
1.3196	8	1•1•15	71.43
1.2520	2	229	75.94
1.2102	3	045	79.06
1.1819	4	1•3•10	81.35

Rubidium iron chloride hydrate, $\text{Rb}_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation at room temperature. Since the material was incongruently soluble, a 1:1 molar aqueous solution of RbCl and FeCl_3 was prepared with some additional HCl . The first crystals formed were used.

Color

Deep reddish orange

Structure

Orthorhombic, Pmnb (62), $Z = 4$, isostructural with $\text{K}_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ and $(\text{NH}_4)_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$. The structure of $\text{K}_2\text{FeCl}_5 \cdot \text{H}_2\text{O}$ was determined by Bellanca [1947].

NBS lattice constants of this sample:

$$\begin{aligned} a &= 9.923(3) \text{ \AA} \\ b &= 13.836(4) \\ c &= 7.092(2) \end{aligned}$$

Volume \AA^3
973.8 \AA^3

Density

(calculated) 2.879 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 1.7(2)$$

Reference

Bellanca, A., (1947). *Rec. Sci. Reconstr.* 17, 1360.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$
6.92	6	020	12.78
6.31	3	011	14.02
5.78	30	101	15.33
5.68	30	120	15.58
5.34	4	111	16.60
4.960	8	200,021	17.87
3.904	8	211	22.76
3.870	4	031	22.96
3.602	4	131	24.70
3.504	50	221	25.40
3.462	25	040	25.71
3.436	20	012	25.91
3.109	17	041	28.69
3.050	30	231	29.26
3.006	8	122	29.70
2.996	7	301	29.80
2.885	25	202	30.97
2.836	90	240	31.52
2.826	100	212	31.63
2.814	70	032	31.77
2.635	8	241	33.99
2.479	55	400,042	36.21
2.403	3	142	37.40
2.308	2	411,060	38.99
2.238	3	023	40.26
2.218	2	421	40.65
2.180	18	052	41.38
2.130	6	152	42.40
2.108	7	213	42.87
2.089	2	431	43.28
2.058	5	133	43.96
2.010	14	412	45.06
2.004	15	261	45.20
1.997	9	252	45.38
1.940	12	441	46.79
1.936	14	233	46.88
1.912	7	501	47.51
1.860	15	432	48.92
1.820	3	352	50.07
1.800	2	262	50.66
1.776	4	333	51.41
1.773	5	004	51.50
1.758	8	014	51.97
1.753	13	442	52.13
1.730	6	080	52.88
1.698	3	413	53.96
1.679	6	081,522	54.61
1.6696	4	204,362	54.95
1.6552	5	034	55.47
1.6378	12	452	56.11

Rubidium lead chromium oxide, $\text{Rb}_2\text{Pb}(\text{CrO}_4)_2$

Sample

The sample was prepared by melting a mixture of Rb_2CrO_4 and PbCrO_4 , at about 730 °C.

Color

Slight orange yellow

Structure

Hexagonal, $\bar{R}3m(166)$, $Z = 3$, isostructural with $\text{Sr}_3(\text{PO}_4)_2$ and many double chromates, sulfates, and selenates [Schwarz, 1966]. The structure of $(\text{NH}_4)_2\text{Pb}(\text{SO}_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

$$a = 5.8037(4) \text{ \AA}$$

$$c = 21.827(3)$$

Volume

$$636.70 \text{ \AA}^3$$

Density

(calculated) 4.773 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 5.3(3)$$

Additional pattern

1. PDF card 19-1077 [Schwarz, 1966].

References

Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 344, 41.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. 25 \pm 1 °C			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
d (Å)	I	hkl	2 θ (°)
7.273	12	003	12.16
4.897	25	101	18.10
4.567	10	012	19.42
3.699	9	104	24.04
3.638	4	006	24.45
3.296	100	015	27.03
2.904	75	110	30.76
2.696	7	113	33.21
2.650	2	107	33.80
2.497	5	021	35.93
2.426	5	009	37.03
2.283	13	024	39.43
2.270	12	116	39.68
2.178	25	205	41.43
2.002	17	1 \cdot 0 \cdot 10	45.26
1.957	2	027	46.34
1.892	5	211	48.04
1.871	3	122	48.63
1.861	5	119	48.89
1.849	1	208	49.24
1.819	1	0 \cdot 0 \cdot 12	50.12
1.794	2	214	50.85
1.742	18	125	52.49
1.675	8	300	54.75
1.648	5	0 \cdot 2 \cdot 10	55.73
1.632	1	303	56.32
1.558	2	2 \cdot 0 \cdot 11	59.26
1.5216	2	306	60.83
1.4889	2	0 \cdot 1 \cdot 14	62.31
1.4546	7	0 \cdot 0 \cdot 15	63.95
1.4506	6	220	64.15
1.4329	8	2 \cdot 1 \cdot 10	65.04
1.3912	2	131	67.24
1.3784	2	309	67.95
1.3720	2	1 \cdot 2 \cdot 11	68.31
1.3507	1	134	69.54
1.3276	5	315	70.93
1.3008	5	1 \cdot 1 \cdot 15	72.62
1.2447	1	229	76.46
1.2242	1	404	77.99
1.2074	3	045	79.28
1.1747	3	1 \cdot 3 \cdot 10	81.95
1.1519	<1	321	83.94
1.1149	2	235	87.41
1.0987	3	3 \cdot 0 \cdot 15	89.03
1.0969	3	410	89.22

Sodium magnesium sulfate hydrate (loeweite), $\text{Na}_{12}\text{Mg}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$

Sample

The sample was prepared by evaporation of an aqueous solution of a 6:7 molar ratio of Na_2SO_4 and MgSO_4 at 95 °C. The precipitate was filtered off while the solution was hot. The composition of this phase was originally given as $\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 2.5\text{H}_2\text{O}$. It was corrected by Kühn and Ritter [1958]. The sample contained about 15% of bloedite [$\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$]. This pattern has been confirmed by computer calculation using structure data from Fang and Robinson [1970]. The sample was colorless.

Intensities

The intensities given in the table have been calculated from the data of Fang and Robinson [1970], and thus represent the intensities which would be obtained from a sample free from bloedite.

Structure

Hexagonal, $R\bar{3}$ (148), $Z = 3$, isostructural with $\text{Na}_{12}\text{Mn}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$ [Schneider and Zemann, 1959]. The structure of loeweite was determined by Fang and Robinson [1970].

NBS lattice constants of this sample:

$$a = 18.866(2) \text{ \AA}$$

$$c = 13.434(2)$$

A least squares refinement based on 43 unique reflections free from bloedite gave lattice constants which did not differ from those above by more than 0.005 Å.

Volume

$$4140.9 \text{ \AA}^3$$

Density

$$(\text{calculated}) 2.364 \text{ g/cm}^3$$

Reference intensity

$$I/I_{\text{corundum}} = 0.56(3)$$

Additional patterns

1. PDF card 21-1139 [Madsen, 1966]
2. PDF card 24-1107 [Heide, Min. Inst. Jena, 1967]. This pattern has the formula incorrectly given as $\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 2.5\text{H}_2\text{O}$.

References

- Fang, J. H., and Robinson, P. D., (1970). Am. Mineralogist 55, 378.
- Kühn, R., and Ritter, K.-H. (1958). Kali Steinsalz 2, 238.
- Madsen, B. M., (1966). U. S. Geol. Surv. Prof. Pap. 550B, 125.
- Schneider, W. (1960). Z. Anorg. Allg. Chem. 303, 113.
- Schneider, W., and Zemann, J. (1959). Beitr. Mineral. Petrogr. 6, 201.

CuK α_1 $\lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$			
Internal standard Ag, $a = 4.08651 \text{ \AA}$			
$d(\text{Å})$	I	hkl	$2\theta(^\circ)$
10.37	100	101	8.52
9.42	18	110	9.38
6.98	26	021	12.68
6.21	14	012	14.26
5.61	28	211	15.78
5.45	32	300	16.26
5.19	5	202	17.07
4.55	8	122	19.49
4.471	10	003	19.84
4.294	65	131	20.67
4.046	62	113	21.95
3.904	2	401	22.76
3.759	31	312	23.65
3.612	9	321	24.63
3.563	4	410	24.97
3.493	2	042	25.48
3.458	52	303	25.74
3.277	45	232	27.19
3.251	23	223	27.41
3.175	41	051	28.08
3.144	10	330	28.36
3.109	4	024	28.69
3.012	6	241	29.64
2.949	3	214	30.28
2.942	21	502	30.36
2.868	22	511	31.16
2.806	17	422	31.87
2.790	23	413	32.06
2.723	22	600	32.86
2.698	47	134	33.18
2.635	15	431	34.00
2.617	17	520	34.24
2.552	1	205	35.14
2.499	1	324	35.90
2.494	3	342	35.98
2.451	10	161	36.64
2.356	5	440	38.16
2.343	1	054	38.39
2.335	5	612	38.52
2.311	4	315	38.94
2.273	1	244	39.62
2.259	2	523	39.87
2.211	15	514	40.78
2.206	15	072	40.87
2.180	6	116	41.39
2.163	3	710	41.72
2.097	2	434	43.10
2.070	9	306	43.69
2.066	11	541	43.78
2.023	16	226	44.76

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$
1.999	8	452	45.34
1.954	4	802	46.43
1.917	8	354	47.38
1.900	4	345	47.84
1.896	4	416	47.95
1.870	3	633	48.65
1.856	1	461	49.03
1.839	6	182	49.54
1.833	4	217	49.69
1.805	4	642	50.51
1.783	3	820	51.18
1.776	6	544	51.42
1.761	3	075	51.87
1.739	8	553,407	52.60
1.716	2	274	53.34
1.708	3	327	53.61
1.699	5	191	53.92
1.694	4	740	54.08
1.6821	3	903	54.51
1.6702	2	018	54.93
1.6557	8	823,057	55.45
1.6503	8	455	55.65
1.6448	6	208	55.85
1.6362	5	464	56.17
1.6301	6	247	56.40
1.6100	5	832	57.17
1.5869	4	0•10•2	58.08
1.5750	5	318	58.56
1.5576	2	185	59.28

Sodium manganese sulfate hydrate, $\text{Na}_{12}\text{Mn}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$

Sample

The sample was prepared by evaporation of an aqueous solution of 4:3 molar mixture of Na_2SO_4 and MnSO_4 at 95 °C. The crystals were filtered off while the solution was hot.

Color

Pale pink

Optical data

Uniaxial (—), $N_e = 1.501$, $N_o = 1.520$

Structure

Hexagonal, $R\bar{3}$ (148), $Z = 3$, isostructural with $\text{Na}_{12}\text{Mg}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$ (loeweite). The structure has been studied by Schneider [1960].

NBS lattice constants of this sample:

$a = 19.126(2) \text{ \AA}$
 $b = 13.529(3) \text{ \AA}$

Volume

4285.7 \AA^3

Density

(calculated) 2.533 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 0.66(7)$

Reference

Schneider, W. (1960). Z. Anorg. Allg. Chem. 303, 113.

$\text{CuK}\alpha_1 \lambda = 1.540598 \text{ \AA}$; temp. $25 \pm 1 \text{ }^\circ\text{C}$

Internal standard Si, $a = 5.43088 \text{ \AA}$

d (Å)	I	hkl	2θ (°)
10.47	55	101	8.44
9.57	25	110	9.23
7.07	85	021	12.51
6.25	35	012	14.15
5.683	30	211	15.58
5.525	30	300	16.03
4.784	20	220	18.53
4.595	25	122	19.30
4.510	35	003	19.67
4.350	80	131	20.40
4.079	70	113	21.77
3.803	16	312	23.37
3.660	30	321	24.30
3.616	14	410	24.60
3.531	14	042	25.21
3.494	80	303	25.47
3.312	90	104,232	26.90
3.282	18	223	27.15
3.218	70	051	27.70
3.189	18	330	27.96

d (Å)	I	hkl	2θ (°)
3.132	11	024	28.48
3.051	7	241	29.25
2.977	35	214,502	29.99
2.907	55	511	30.73
2.843	40	422	31.44
2.820	45	413	31.70
2.760	50	600	32.41
2.723	100	134,152	32.86
2.669	9	015,431	33.55
2.651	30	520	33.78
2.603	8	333	34.43
2.527	10	324,342	35.50
2.483	9	125,161	36.14
2.391	9	440	37.59
2.367	25	054,612	37.99
2.329	17	315,351	38.62
2.285	5	523	39.40
2.265	8	045,621	39.76
2.254	18	006	39.96
2.233	55	514,072	40.36
2.194	11	116,710	41.11
2.122	6	434	42.57
2.113	6	443	42.75
2.095	20	505,541	43.15
2.089	16	306,630	43.28
2.046	17	425,081	44.23
2.039	30	226	44.39
2.022	15	164,452	44.78
2.001	6	155,271	45.29
1.979	8	802	45.81
1.973	9	713	45.95
1.938	19	354,722	46.83
1.920	14	107,345	47.31
1.913	10	416,550	47.48
1.893	10	633	48.01
1.882	4	027,461	48.33
1.864	6	182	48.83
1.846	6	615,731	49.32
1.841	8	336,900	49.48
1.829	9	642	49.83
1.796	10	544,372	50.80
1.781	12	137,075	51.26
1.761	15	553	51.89
1.736	4	274	52.67
1.722	13	327,191	53.15
1.717	13	526,740	53.31
1.704	6	903	53.75
1.681	16	814,562	54.54
1.678	14	823	54.66
1.670	12	057,455	54.94
1.657	12	208,464	55.40
1.620	8	921,725 +	56.78
1.608	10	0·10·2	57.24
1.604	7	743	57.39
1.586	12	318,292	58.10

Acetanilide, $C_6H_5NHCOCH_3$

Synonym

N - phenylacetamide

Structure

Orthorhombic, Pbc_a (61), Z = 8. The structure was determined by Brown and Corbridge [1954] and refined by Brown [1966].

Atom positions

All atoms were in general positions.

Lattice constants

a = 19.641 Å

b = 9.483

c = 7.979

(published values: a = 19.640, b = 9.483,

c = 7.979 [Brown and Corbridge, 1954]).

CD cell: a = 9.483, b = 19.641, c = 7.979,

space group Pcab; a/b = 0.4828, c/b = 0.4063

Volume

1486. Å³

Density

(measured) 1.206 g/cm³

(calculated) 1.208 g/cm³

Thermal parameters

Isotropic: overall B = 5.0

Scattering factors

C⁰, H⁰, N⁰, O⁰ [International Tables, 1962]

Scale factors (integrated intensities)

$\gamma = 1.471 \times 10^{-3}$

I/I_c (calculated) = 0.50

Additional pattern

1. PDF card 18-1501 [Billig, B. and Greenberg, B., Polytechnic Inst. of Brooklyn]

References

Brown, C. J. and Corbridge, D. E. C. (1954). Acta Crystallogr. 7, 711.

Brown, C. J. (1966). Acta Crystallogr. 21, 442.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d (Å)	I	hkl	2θ (°) λ = 1.540598 Å
9.82	100	2 0 0	9.00
6.82	38	2 1 0	12.98
5.82	81	1 1 1	15.20
5.18	31	2 1 1	17.10
4.91	3	4 0 0	18.06
4.74	6	0 2 0	18.72
4.46	26	3 1 1	19.88
4.36	27	4 1 0	20.36
4.27	5	2 2 0	20.80
4.07	40	0 2 1	21.80
3.99	58	1 2 1	22.26
3.91	29	1 0 2	22.74
3.82	9	4 1 1	23.24
3.76	36	2 2 1	23.62
3.70	73	2 0 2	24.06
3.61	25	1 1 2	24.62
3.44	47	2 1 2	25.86
3.41	8	3 0 2	26.12
3.30	6	5 1 1	26.98
3.20	17	3 1 2	27.82
3.09	7	4 0 2*	28.84
3.05	15	0 2 2	29.24
3.02	30	1 2 2	29.60
2.884	1	6 1 1	30.98
2.815	6	2 3 1	31.76
2.766	4	3 2 2	32.34
2.693	3	6 2 0	33.24
2.687	3	5 1 2	33.32
2.657	2	4 3 0	33.70
2.592	6	4 2 2	34.58
2.539	4	1 1 3	35.32
2.532	4	6 0 2	35.42
2.478	3	2 1 3	36.22
2.445	1	6 1 2	36.72
2.410	2	5 2 2	37.28
2.377	5	8 1 0	37.82
2.353	1	5 3 1	38.22
2.311	3	7 2 1*	38.94
2.304	4	1 2 3	39.06
2.295	5	7 0 2	39.22
2.273	6	6 3 0*	39.62
2.258	2	2 2 3*	39.90
2.214	2	2 4 1	40.72
2.186	4	3 2 3*	41.26
2.097	1	4 2 3	43.10
2.065	2	7 2 2	43.80
2.055	2	9 1 1	44.02
2.024	2	1 3 3	44.74
1.967	1	5 4 1*	46.12
1.943	3	3 3 3*	46.72

Acetanilide, $C_6H_5NHC(=O)CH_3$ - (Continued)

Calculated Pattern (Peak heights)					
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å	
1.919	3	6 4 0*	47.32		
1.915	3	9 0 2*	47.44		
1.892	2	7 1 3*	48.06		
1.884	2	8 3 1*	48.28		
1.880	2	4 3 3*	48.38		
1.870	3	10 1 1*	48.64		
1.838	1	0 2 4*	49.56		
1.813	1	2 5 1*	50.28		
1.808	2	2 2 4*	50.44		
1.771	4	3 2 4*	51.58		
1.748	2	5 1 4	52.30		
1.744	2	8 3 2	52.42		
1.708	1	3 4 3*	53.60		
1.668	1	10 3 0	55.00		
1.664	1	2 3 4*	55.16		
1.658	1	3 5 2	55.38		

Calculated Pattern (Integrated)					
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å	
9.82	100	2 0 0	9.00		
6.82	39	2 1 0	12.97		
5.83	85	1 1 1	15.18		
5.18	33	2 1 1	17.09		
4.91	3	4 0 0	18.05		
4.74	6	0 2 0	18.70		
4.47	28	3 1 1	19.87		
4.36	29	4 1 0	20.35		
4.27	5	2 2 0	20.79		
4.08	43	0 2 1	21.79		
3.99	61	1 2 1	22.26		
3.99	4	0 0 2	22.27		
3.91	31	1 0 2	22.73		
3.83	8	4 1 1	23.23		
3.76	39	2 2 1	23.61		
3.70	82	2 0 2	24.06		
3.61	28	1 1 2	24.61		
3.46	2	3 2 1	25.73		
3.44	53	2 1 2	25.85		
3.41	1	4 2 0	26.11		
3.41	5	3 0 2	26.14		
3.30	6	5 1 1	26.97		
3.21	20	3 1 2	27.80		
3.10	4	4 0 2	28.81		
3.09	3	6 1 0	28.83		
3.05	16	0 2 2	29.23		
3.02	34	1 2 2	29.59		
3.01	2	2 3 0	29.67		
2.885	1	6 1 1	30.97		
2.828	2	5 2 1	31.61		

Calculated Pattern (Integrated)					
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å	
2.815	6	2 3 1	31.76		
2.767	4	3 2 2	32.33		
2.694	3	6 2 0	33.23		
2.685	1	5 1 2	33.35		
2.658	2	4 3 0	33.69		
2.592	8	4 2 2	34.57		
2.552	1	6 2 1	35.13		
2.549	1	7 1 1	35.17		
2.539	4	1 1 3	35.32		
2.531	3	6 0 2	35.44		
2.478	3	2 1 3	36.22		
2.445	1	6 1 2	36.73		
2.410	2	5 2 2	37.27		
2.377	5	8 1 0	37.82		
2.371	1	0 4 0	37.92		
2.353	1	5 3 1	38.22		
2.317	1	3 3 2	38.83		
2.311	2	7 2 1	38.94		
2.304	2	1 2 3	39.07		
2.295	5	7 0 2	39.22		
2.278	1	8 1 1	39.53		
2.274	4	6 3 0	39.60		
2.273	2	0 4 1	39.63		
2.258	1	2 2 3	39.90		
2.257	1	1 4 1	39.90		
2.214	3	2 4 1	40.72		
2.187	2	6 3 1	41.25		
2.186	3	3 2 3	41.26		
2.145	1	5 1 3	42.09		
2.097	1	4 2 3	43.09		
2.066	3	7 2 2	43.79		
2.055	2	9 1 1	44.03		
2.024	3	1 3 3	44.73		
1.967	1	5 4 1	46.11		
1.943	2	3 3 3	46.70		
1.942	2	1 1 4	46.73		
1.923	1	10 1 0	47.22		
1.920	2	6 4 0	47.30		
1.915	1	9 0 2	47.45		
1.893	1	6 2 3	48.03		
1.891	2	7 1 3	48.06		
1.884	1	8 3 1	48.26		
1.880	1	4 3 3	48.38		
1.877	1	9 1 2	48.47		
1.871	1	3 1 4	48.63		
1.870	2	10 1 1	48.66		
1.839	1	0 2 4	49.54		
1.813	1	2 5 1	50.27		
1.807	1	2 2 4	50.46		
1.776	1	3 5 1	51.41		

Acetanilide, $C_6H_5NHCOCH_3$ - (Continued)

Calculated Pattern (Integrated)					
$d(\text{\AA})$	I	hkl			$2\theta(^{\circ})$
					$\lambda = 1.540598\text{\AA}$
1.772	2	8	1	3	51.53
1.770	3	3	2	4	51.59
1.763	1	1	4	3	51.83
1.748	2	5	1	4	52.29
1.744	1	8	3	2	52.43
1.722	1	4	2	4	53.15
1.708	2	3	4	3	53.60
1.668	1	10	3	0	55.00
1.663	1	2	3	4	55.20
1.657	1	3	5	2	55.40
1.633	1	10	3	1	56.29

Allobarbitol, $C_{10}H_{12}N_2O_3$

Synonyms

5,5 - diallylbarbituric acid, Dial

Structure

Monoclinic, C2/c (15), Z = 8. The structure was determined by Escobar [1975].

Atom positions

There was some disorder in the structure, with one carbon randomly occupying 2 sites in the proportion of 4 to 1. All other atoms were in general positions [ibid.].

Lattice constants

a = 14.570 Å

b = 7.289

c = 20.618

$\beta = 99.83^\circ$

(published values: a = 14.569(6), b = 7.289(4), c = 20.617(7), $\beta = 99.83(4)^\circ$ [Escobar, 1975]).

CD cell: a = 20.618, b = 7.289, c = 14.570, $\beta = 99.83^\circ$, space group A2/a; a/b = 2.8286, c/b = 1.9989

Volume

2157.5 Å³

Density

(measured) 1.278

(calculated) 1.282

Thermal parameters

Isotropic: overall B = 4.0

Scattering factors

C⁰, H⁰, N⁰, O⁰ [International Tables, 1962]

Scale factors (integrated intensities)

$\gamma = 1.627 \times 10^{-3}$

I/I_c (calculated) = 0.65

Additional pattern

1. PDF card 5-158 [Huang, 1951]

References

Escobar, C. (1975). Acta Crystallogr. B31, 1059.

Huang, T.-Y. (1951). Acta Pharm. Int. 2, 43.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)					
d (Å)	I	hkl			2 θ (°)
					$\lambda = 1.540598\text{Å}$
10.16	6	0	0	2	8.70
7.17	3	2	0	0	12.34
6.50	100	1	1	0	13.62
6.39	52	-2	0	2	13.84
6.05	51	1	1	1	14.62
5.68	16	-1	1	2	15.60
5.43	26	2	0	2	16.30
5.29	25	1	1	2	16.76
5.08	44	0	0	4	17.46
4.88	33	-1	1	3	18.18
4.52	2	-2	0	4	19.62
4.16	6	-1	1	4	21.34
4.03	34	-3	1	1	22.02
4.00	14	3	1	0	22.20
3.917	3	-3	1	2	22.68
3.821	7	3	1	1	23.26
3.681	12	-3	1	3	24.16
3.642	22	0	2	0	24.42
3.587	10	0	2	1	24.80
3.553	6	3	1	2	25.04
3.386	6	-3	1	4	26.30
3.329	4	1	1	5	26.76
3.285	14	-2	0	6	27.12
3.248	52	2	2	0*	27.44
3.216	15	4	0	2*	27.72
3.169	5	2	2	1*	28.14
3.102	6	-1	1	6	28.76
3.026	11	2	2	2*	29.50
2.944	18	3	1	4	30.34
2.877	2	2	0	6	31.06
2.845	2	2	2	3	31.42
2.788	2	-3	1	-6	32.08
2.714	9	4	0	4*	32.98
2.692	4	-5	1	2	33.26
2.671	3	5	1	0	33.52
2.639	6	-2	2	5*	33.94
2.595	1	5	1	1	34.54
2.555	4	-4	2	2	35.10
2.534	5	-2	0	8	35.40
2.481	2	0	2	6	36.18
2.447	3	2	2	5	36.70
2.429	5	-1	1	8	36.98
2.420	5	3	1	6	37.12
2.405	3	-4	2	4	37.36
2.399	3	1	3	0	37.46
2.388	3	-1	3	1	37.64
2.371	4	1	3	1	37.92
2.346	3	-1	3	2	38.34
2.323	2	-6	0	4	38.74
2.317	2	1	3	2	38.84

Allobarbitol, C₁₀H₁₂N₂O₃ - (Continued)

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
2.275	1	2 0 8*	39.58	
2.245	1	6 0 2	40.14	
2.223	2	5 1 4	40.54	
2.184	2	-1 1 9	41.30	
2.179	2	4 2 4	41.40	
2.172	4	-3 3 1	41.54	
2.167	4	3 3 0	41.64	
2.082	2	1 1 9*	43.42	
2.046	2	-4 2 7	44.24	
2.033	1	0 0 10*	44.54	
2.006	1	-5 1 8	45.16	
2.000	2	-6 2 3*	45.30	
1.984	1	-7 1 3*	45.68	
1.959	1	-6 2 4	46.32	
1.952	1	-7 1 4*	46.48	
1.923	1	-4 2 8*	47.22	
1.913	1	-4 0 10*	47.48	
1.861	1	-5 3 2	48.90	
1.853	1	3 3 5*	49.12	
1.848	1	6 2 3	49.26	
1.843	1	-7 1 6	49.42	
1.822	1	1 3 7*	50.02	
1.813	1	4 2 7*	50.30	
1.791	2	-8 0 4*	50.96	
1.766	2	2 4 0	51.72	
1.746	1	7 1 4	52.36	
1.714	1	-2 0 12*	53.40	
1.710	1	-8 0 6*	53.54	
1.690	1	-2 4 4*	54.22	
1.683	1	5 3 4	54.46	
1.630	1	-4 4 1*	56.42	
1.624	2	-4 4 2*	56.62	
1.608	1	-4 4 3*	57.24	
1.595	1	2 4 5*	57.76	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
10.16	6	0 0 2	8.70	
7.18	3	2 0 0	12.32	
6.50	100	1 1 0	13.61	
6.40	45	-2 0 2	13.83	
6.33	4	-1 1 1	13.97	
6.06	53	1 1 1	14.62	
5.68	16	-1 1 2	15.60	
5.44	27	2 0 2	16.28	
5.29	26	1 1 2	16.74	
5.08	47	0 0 4	17.45	
4.88	36	-1 1 3	18.16	
4.53	3	-2 0 4	19.60	
4.16	6	-1 1 4	21.34	
4.04	37	-3 1 1	22.01	
4.00	11	3 1 0	22.21	
3.917	3	-3 1 2	22.68	
3.823	8	3 1 1	23.25	
3.682	12	-3 1 3	24.15	
3.645	25	0 2 0	24.40	
3.587	11	0 2 1	24.80	
3.553	6	3 1 2	25.04	
3.386	6	-3 1 4	26.30	
3.331	3	1 1 5	26.74	
3.286	14	-2 0 6	27.11	
3.250	37	2 2 0	27.42	
3.248	23	-2 2 1	27.44	
3.247	1	3 1 3	27.45	
3.216	13	4 0 2	27.72	
3.209	3	0 2 3	27.78	
3.171	3	2 2 1	28.12	
3.167	1	-2 2 2	28.16	
3.103	7	-1 1 6	28.75	
3.028	10	2 2 2	29.48	
3.022	4	-2 2 3	29.53	
2.961	7	0 2 4	30.16	
2.945	21	3 1 4	30.33	
2.878	3	2 0 6	31.04	
2.845	2	2 2 3	31.42	
2.788	2	-3 1 6	32.08	
2.730	1	-1 1 7	32.78	
2.720	7	4 0 4	32.90	
2.713	5	0 2 5	32.99	
2.705	1	-5 1 1	33.10	
2.704	1	-4 0 6	33.10	
2.691	3	-5 1 2	33.27	
2.671	2	5 1 0	33.52	
2.646	2	2 2 4	33.85	
2.639	5	-2 2 5	33.94	
2.596	1	5 1 1	34.53	
2.554	5	-4 2 2	35.10	

Calculated Pattern (Integrated)					
d (Å)	I	hkl			2θ (°) λ = 1.540598 Å
2.534	6	-2	0	8	35.40
2.481	2	0	2	6	35.18
2.447	3	2	2	5	36.69
2.430	5	-1	1	8	36.97
2.420	4	3	1	6	37.13
2.404	3	-4	2	4	37.37
2.396	1	1	3	0	37.51
2.387	2	-1	3	1	37.65
2.371	4	1	3	1	37.91
2.347	3	-1	3	2	38.33
2.323	2	-6	0	4	38.74
2.317	1	1	3	2	38.84
2.275	1	2	0	8	39.58
2.245	1	6	0	2	40.14
2.223	2	5	1	4	40.55
2.185	2	-1	1	9	41.28
2.180	1	4	2	4	41.39
2.172	5	-3	3	1	41.54
2.166	1	3	3	0	41.66
2.083	1	1	1	9	43.41
2.080	1	-2	2	8	43.46
2.046	2	-4	2	7	44.23
2.031	1	0	0	10	44.57
2.006	1	-5	1	8	45.15
2.000	1	6	2	0	45.30
1.997	1	-6	2	3	45.37
1.985	1	-7	1	3	45.67
1.959	1	-6	2	4	46.32
1.923	1	-4	2	8	47.24
1.861	1	-5	3	2	48.90
1.848	1	6	2	3	49.27
1.842	1	-7	1	6	49.43
1.826	1	5	1	7	49.90
1.791	2	-8	0	4	50.96
1.766	2	2	4	0	51.71
1.746	1	7	1	4	52.37
1.714	1	-2	0	12	53.40
1.690	1	-2	4	4	54.22
1.683	1	5	3	4	54.47
1.670	1	-1	1	12	54.94
1.630	1	-4	4	1	56.42
1.624	1	-4	4	2	56.63
1.608	1	-4	4	3	57.23
1.595	1	2	4	5	57.74

Calcium carbonate, aragonite, CaCO_3

Structure

Orthorhombic, Pnma (62), $Z = 4$. The structure was determined by Bragg [1924] and refined by de Villiers [1971]. Aragonite is isostructural with strontianite (SrCO_3) and witherite (BaCO_3) [de Villiers, 1971].

Atom positions

4(c) 4 calcium
4(c) 4 carbon
4(c) 4 oxygen(1)
8(d) 8 oxygen(2)

Polymorphism

There are 2 hexagonal polymorphs, calcite and vaterite; the 3 forms may coexist in synthetic samples.

Lattice constants

$a = 5.740(1)$
 $b = 4.9614(6)$
 $c = 7.966(1)$
This cell was refined from NBS data [Swanson, Fuyat and Ugrinic, 1954, and on PDF card 5-453]

CD cell: $a=5.740(1)$, $b=7.966(1)$, $c=4.9614(6)$,
space group, Pnam, $a/b = 0.7206$, $c/b = 0.6228$

Volume \AA^3
226.9

Density

(calculated) 2.931 g/cm^3

Thermal parameters

Anisotropic [de Villiers, 1971]

Scattering factors

Ca^{2+} , C^0 [International Tables, 1962]
 O^{2-} [Suzuki, 1960]

Scale factors (integrated intensities)

$\gamma = 0.220 \times 10^{-3}$
 I/I_c (calculated) = 0.98

Additional patterns

1. PDF card 5-453 [Powder Diffraction Data 1976]
2. PDF card 24-25 [Smith et al., 1973]

References

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dards.
Suzuki, T. (1960). Acta Crystallogr. 13, 279.
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de Villiers, J. P. R. (1971). Am. Mineralogist 56,
758.

Calculated Pattern (Peak heights)

d (Å)	I	hkl	2θ (°) λ = 1.540598 Å
4.653	1	1 0 1	19.06
4.211	5	0 1 1	21.08
3.980	2	0 0 2	22.32
3.394	100	1 1 1	26.24
3.271	62	1 0 2	27.24
2.8698	4	2 0 0	31.14
2.7315	11	1 1 2	32.76
2.6995	62	2 0 1	33.16
2.4821	43	2 1 0+	36.16
2.4100	18	1 0 3	37.28
2.3708	42	2 1 1	37.92
2.3411	31	0 1 3	38.42
2.3283	24	2 0 2	38.64
2.1893	15	1 2 1	41.20
2.1682	1	1 1 3	41.62
2.1055	22	0 2 2	42.92
1.9911	6	0 0 4	45.52
1.9771	69	1 2 2	45.86
1.9498	1	2 0 3	46.54
1.8813	34	1 0 4	48.34
1.8769	38	2 2 0	48.46
1.8268	3	2 2 1	49.88
1.8139	28	2 1 3	50.26
1.7591	4	1 1 4	51.94
1.7416	28	3 1 1	52.50
1.7282	11	1 2 3	52.94
1.7246	18	3 0 2	53.06
1.6979	2	2 2 2	53.96
1.6359	2	2 0 4	56.18
1.6296	1	3 1 2	56.42
1.6190	2	0 3 1	56.82
1.5585	6	1 3 1	59.24
1.5350	2	1 0 5	60.24
1.5318	1	2 2 3	60.38
1.5168	1	0 1 5	61.04
1.4991	6	1 2 4	61.84
1.4759	3	1 3 2	62.92
1.4663	7	1 1 5	63.38
1.4329	1	2 3 0+	65.04
1.4121	4	4 0 1	66.12
1.4102	4	2 3 1	66.22
1.4038	4	0 3 3	66.56
1.3786	1	4 1 0	67.94
1.3659	4	2 2 4	68.66
1.3583	5	4 1 1	69.10
1.3501	2	4 0 2	69.58
1.3410	3	2 1 5	70.12
1.3278	2	0 0 6	70.92
1.3055	1	1 2 5	72.32
1.3024	1	4 1 2	72.52

Calcium carbonate, aragonite, CaCO_3 - (Continued)

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
1.2611	6	2 3 3	75.30	
1.2404	7	0 4 0+	76.78	
1.2360	9	3 3 1	77.10	
1.2235	6	4 1 3	78.04	
1.2146	2	2 2 5	78.72	
1.2057	8	3 2 4+	79.42	
1.1937	1	3 3 2	80.38	
1.1888	6	3 1 5	80.78	
1.1706	9	0 2 6	82.30	
1.1643	1	4 0 4	82.84	
1.1598	3	1 4 2	83.24	
1.1470	1	1 2 6	84.38	
1.1385	1	2 4 0	85.16	
1.1359	1	5 0 1	85.40	
1.1333	1	4 1 4	85.64	
1.1318	1	3 3 3	85.78	
1.1269	2	2 4 1	86.24	
1.1251	4	1 3 5	86.42	
1.1164	1	1 0 7	87.26	
1.1075	2	5 1 1	88.14	
1.1031	1	5 0 2+	88.58	
1.0978	1	3 2 5	89.12	
1.0947	2	2 4 2	89.44	
1.0890	1	1 1 7	90.04	
1.0839	1	2 2 6	90.58	
1.0739	1	4 3 1	91.66	
1.0655	2	2 3 5	92.60	
1.0595	1	3 3 4	93.28	
1.0579	1	2 0 7	93.46	
1.0539	1	4 2 4+	93.92	
1.0465	1	2 4 3	94.80	
1.0425	1	4 1 5	95.28	
1.0356	4	1 4 4+	96.12	
1.0330	4	5 2 1	96.44	
1.0180	1	1 2 7+	98.34	
1.0079	4	5 2 2	99.68	
1.0070	3	3 4 2	99.80	
1.0035	4	4 3 3	100.28	
.9986	1	3 2 6	100.96	
.9957	1	0 0 8	101.36	
.9946	1	5 0 4	101.52	
.9884	1	2 4 4	102.40	
.9840	2	3 3 5	103.04	
.9811	2	1 0 8	103.46	
.9795	1	4 2 5	103.70	
.9739	2	2 3 6+	104.54	
.9732	1	2 2 7	104.66	
.9706	2	1 5 1	105.06	
.9648	1	1 4 5	105.96	
.9624	1	1 1 8	106.34	

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
.9596	3	3 1 7	106.78	
.9568	3	6 0 0	107.24	
.9520	1	4 3 4	108.02	
.9497	1	6 0 1	108.40	
.9407	1	2 0 8	109.94	
.9378	1	2 5 0	110.44	
.9365	1	5 3 1	110.68	
.9315	3	2 5 1+	111.58	
.9295	3	0 5 3	111.94	
.9252	1	1 3 7	112.72	
.9231	1	5 2 4	113.12	
.9175	1	1 5 3+	114.18	
.9154	2	5 1 5	114.60	
.9132	2	4 4 2	115.02	
.9123	3	1 2 8	115.20	
.9063	2	0 4 6+	116.40	
.9001	1	6 0 3	117.70	
.8961	1	4 3 5	118.54	
.8926	1	6 2 0	119.30	
.8912	2	2 3 7	119.62	
.8856	2	6 1 3	120.88	
.8843	2	2 5 3	121.18	
.8796	1	2 2 8	122.26	
.8776	2	4 1 7+	122.74	
.8755	2	3 5 1	123.24	
.8712	1	0 1 9+	124.30	
.8643	2	2 4 6	126.06	
.8601	1	3 5 2	127.16	
.8523	1	5 3 4	129.32	
.8489	1	4 4 4	130.30	
.8460	1	6 2 3	131.14	
.8439	1	1 3 8	131.78	
.8419	3	3 3 7	132.40	
.8391	1	4 2 7	133.26	
.8378	1	5 4 1	133.68	
.8360	1	3 5 3	134.26	
.8338	3	2 1 9+	135.00	
.8320	2	3 2 8	135.58	
.8269	1	0 6 0	137.36	
.8243	1	5 4 2	138.30	
.8202	1	6 0 5	139.84	
.8161	1	4 5 0	141.42	
.8157	1	7 0 1	141.58	
.8142	1	6 2 4+	142.20	
.8118	2	4 5 1	143.20	
.8116	2	5 3 5	143.28	
.8096	2	0 6 2	144.14	
.8082	1	2 5 5+	144.76	
.8049	1	7 1 1	146.28	
.8031	1	7 0 2+	147.14	

Calcium carbonate, aragonite, CaCO_3 - (Continued)

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{Å}$
.8017	3	1 6 2	147.82	
.8006	1	2 2 9	148.38	
.7977	1	5 1 7	149.90	
.7966	1	0 0 10	150.46	
.7946	1	2 6 0	151.60	
.7927	1	7 1 2	152.70	
.7906	2	6 3 3	154.00	
.7890	1	1 0 10	155.00	
.7849	2	4 3 7	157.90	
.7834	1	7 0 3	159.00	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{Å}$
4.657	1	1 0 1	19.04	
4.211	5	0 1 1	21.08	
3.983	2	0 0 2	22.30	
3.395	100	1 1 1	26.22	
3.272	62	1 0 2	27.23	
2.8700	4	2 0 0	31.14	
2.7317	10	1 1 2	32.76	
2.7001	65	2 0 1	33.15	
2.4843	34	2 1 0	36.13	
2.4807	18	0 2 0	36.18	
2.4100	18	1 0 3	37.28	
2.3716	45	2 1 1	37.91	
2.3411	31	0 1 3	38.42	
2.3285	21	2 0 2	38.64	
2.1894	16	1 2 1	41.20	
2.1678	1	1 1 3	41.63	
2.1057	24	0 2 2	42.92	
1.9915	4	0 0 4	45.51	
1.9769	79	1 2 2	45.87	
1.9491	1	2 0 3	46.56	
1.8815	34	1 0 4	48.34	
1.8768	21	2 2 0	48.46	
1.8604	1	3 0 1	48.92	
1.8268	2	2 2 1	49.88	
1.8141	32	2 1 3	50.25	
1.7592	4	1 1 4	51.94	
1.7420	33	3 1 1	52.49	
1.7286	8	1 2 3	52.93	
1.7247	15	3 0 2	53.06	
1.6977	3	2 2 2	53.96	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{Å}$
1.6362	3	2 0 4	56.17	
1.6290	1	3 1 2	56.44	
1.6193	2	0 3 1	56.81	
1.5584	7	1 3 1	59.24	
1.5530	1	0 2 4	59.47	
1.5352	2	1 0 5	60.23	
1.5326	1	2 2 3	60.35	
1.5169	1	0 1 5	61.04	
1.4991	7	1 2 4	61.84	
1.4884	1	3 2 1	62.34	
1.4760	4	1 3 2	62.92	
1.4666	8	1 1 5	63.37	
1.4350	1	4 0 0	64.93	
1.4329	1	2 3 0	65.04	
1.4161	1	3 2 2	65.91	
1.4123	4	4 0 1	66.11	
1.4103	3	2 3 1	66.21	
1.4038	4	0 3 3	66.56	
1.3785	1	4 1 0	67.95	
1.3658	4	2 2 4	68.66	
1.3636	1	1 3 3	68.79	
1.3583	6	4 1 1	69.10	
1.3501	2	4 0 2	69.58	
1.3483	1	2 3 2	69.68	
1.3411	3	2 1 5	70.11	
1.3293	1	3 1 4	70.83	
1.3277	2	0 0 6	70.93	
1.3054	1	1 2 5	72.33	
1.3027	1	4 1 2	72.50	
1.2610	8	2 3 3	75.30	
1.2421	3	4 2 0	76.65	
1.2403	7	0 4 0	76.78	
1.2360	10	3 3 1	77.10	
1.2235	7	4 1 3	78.04	
1.2146	2	2 2 5	78.72	
1.2058	9	3 2 4	79.41	
1.2050	4	2 0 6	79.47	
1.1937	1	3 3 2	80.38	
1.1887	7	3 1 5	80.79	
1.1858	1	4 2 2	81.02	
1.1709	1	2 1 6	82.27	
1.1706	11	0 2 6	82.30	
1.1642	1	4 0 4	82.85	
1.1598	4	1 4 2	83.23	
1.1470	1	1 2 6	84.38	
1.1386	1	2 4 0	85.15	
1.1363	1	5 0 1	85.36	
1.1335	1	4 1 4	85.63	
1.1318	1	3 3 3	85.78	
1.1271	2	2 4 1	86.22	

Calcium carbonate, aragonite, CaCO_3 - (Continued)

Calculated Pattern (Integrated)					
d(Å)	I	hkl			2θ(°) λ = 1.540598Å
1.1251	4	1	3	5	86.41
1.1251	1	4	2	3	86.41
1.1163	1	1	0	7	87.27
1.1092	1	0	1	7	87.97
1.1076	3	5	1	1	88.13
1.1031	1	5	0	2	88.58
1.1029	1	1	4	3	88.61
1.0979	1	3	2	5	89.11
1.0947	2	2	4	2	89.44
1.0890	2	1	1	7	90.03
1.0839	2	2	2	6	90.58
1.0740	1	4	3	1	91.66
1.0654	2	2	3	5	92.61
1.0594	1	3	3	4	93.28
1.0579	1	2	0	7	93.46
1.0539	1	4	2	4	93.92
1.0537	1	5	0	3	93.94
1.0528	1	0	4	4	94.05
1.0464	1	2	4	3	94.80
1.0425	2	4	1	5	95.28
1.0356	5	1	4	4	96.12
1.0346	2	2	1	7	96.24
1.0330	2	5	2	1	96.43
1.0189	1	1	3	6	98.23
1.0180	1	1	2	7	98.35
1.0079	4	5	2	2	99.68
1.0070	3	3	4	2	99.81
1.0035	4	4	3	3	100.28
.9985	1	3	2	6	100.97
.9957	1	0	0	8	101.35
.9946	2	5	0	4	101.52
.9884	1	2	4	4	102.40
.9840	2	3	3	5	103.04
.9811	2	1	0	8	103.47
.9796	1	4	2	5	103.69
.9745	1	4	0	6	104.45
.9739	2	2	3	6	104.55
.9731	1	2	2	7	104.67
.9705	2	1	5	1	105.07
.9699	1	5	2	3	105.17
.9648	1	1	4	5	105.96
.9625	1	1	1	8	106.33
.9596	5	3	1	7	106.78
.9567	3	6	0	0	107.26
.9520	1	4	3	4	108.02
.9498	1	6	0	1	108.38
.9407	1	2	0	8	109.93
.9384	1	4	4	0	110.34
.9378	1	2	5	0	110.45
.9365	2	5	3	1	110.67

Calculated Pattern (Integrated)					
d(Å)	I	hkl			2θ(°) λ = 1.540598Å
.9319	2	4	4	1	111.49
.9314	1	5	0	5	111.59
.9314	2	2	5	1	111.59
.9295	2	0	5	3	111.94
.9252	1	1	3	7	112.72
.9232	1	5	2	4	113.11
.9224	1	3	4	4	113.25
.9175	1	1	5	3	114.18
.9154	2	5	1	5	114.59
.9134	1	4	4	2	114.99
.9128	1	2	5	2	115.10
.9123	4	1	2	8	115.20
.9071	1	4	2	6	116.26
.9064	2	0	4	6	116.40
.9000	1	6	0	3	117.71
.8961	2	4	3	5	118.54
.8926	1	6	2	0	119.31
.8912	2	2	3	7	119.63
.8870	1	6	2	1	120.54
.8856	3	6	1	3	120.88
.8843	3	2	5	3	121.17
.8833	1	3	0	8	121.40
.8796	2	2	2	8	122.26
.8777	1	1	5	4	122.72
.8776	1	4	1	7	122.74
.8755	3	3	5	1	123.24
.8748	1	1	0	9	123.42
.8714	1	0	1	9	124.26
.8710	1	6	2	2	124.35
.8696	1	3	1	8	124.70
.8643	4	2	4	6	126.06
.8623	1	6	0	4	126.58
.8601	1	3	5	2	127.17
.8523	1	5	3	4	129.31
.8496	1	6	1	4	130.10
.8489	1	4	4	4	130.31
.8461	1	6	2	3	131.13
.8458	1	2	0	9	131.21
.8438	1	1	3	8	131.82
.8423	1	0	5	5	132.28
.8419	6	3	3	7	132.41
.8396	1	4	3	6	133.11
.8391	2	4	2	7	133.27
.8378	1	5	4	1	133.67
.8361	1	3	5	3	134.25
.8338	5	2	1	9	135.00
.8334	2	1	5	5	135.14
.8321	3	3	2	8	135.55
.8297	1	1	4	7	136.36
.8281	1	6	3	0	136.93

Calcium carbonate, aragonite, CaCO_3 - (Continued)

Calculated Pattern (Integrated)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
.8269	1	0 6 0	137.36	
.8250	1	1 2 9	138.04	
.8243	2	5 4 2	138.30	
.8237	1	6 3 1	138.53	
.8202	1	6 0 5	139.84	
.8162	1	4 5 0	141.40	
.8157	1	7 0 1	141.59	
.8145	1	6 2 4	142.07	
.8142	1	1 6 1	142.21	
.8119	4	4 5 1	143.15	
.8115	4	5 3 5	143.31	
.8096	1	0 6 2	144.13	
.8086	1	4 4 5	144.61	
.8082	1	5 0 7	144.77	
.8082	1	2 5 5	144.77	
.8056	1	3 5 4	145.96	
.8049	1	2 4 7	146.28	
.8049	2	7 1 1	146.29	
.8032	2	7 0 2	147.11	
.8031	1	5 4 3	147.15	
.8017	7	1 6 2	147.82	
.8005	1	2 2 9	148.40	
.7995	1	4 5 2	148.91	
.7977	3	5 1 7	149.89	
.7966	1	0 0 10	150.47	
.7946	3	2 6 0	151.60	
.7930	1	3 1 9	152.52	
.7928	1	7 1 2	152.61	
.7905	5	6 3 3	154.01	
.7890	2	1 0 10	154.98	
.7848	5	4 3 7	157.90	
.7835	1	7 0 3	158.94	

Calcium oxide (lime), CaO

Structure

Cubic, Fm3m (225), Z = 4, isostructural with NaCl [Davey and Hoffman, 1920].

Atom positions

4(a) 4 calcium
4(b) 4 oxygen

Lattice constants

a = 4.8108 Å
(published value, 4.8105 [Swanson and Tatge, 1953, and on PDF card 4-777])

Volume

111.34 Å³

Density

(calculated) 3.345 g/cm³

Thermal parameters

Isotropic: calcium B = 0.5; oxygen B = 1.0

Scattering factors

O²⁻ [Suzuki, 1960]

Ca²⁺ [International Tables, 1962]

Scale factors (integrated intensities)

$\gamma = 0.611 \times 10^{-3}$

I/I_c (calculated) = 4.56

Additional pattern

1. PDF card 4-777 [Powder Diffraction Data, 1976].

References

Davey, W. P. and Hoffman, E. O. (1920). Phys. Rev. 15, 333.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 204.

Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976). (The Joint Committee on Powder Diffraction Standards, Swarthmore, PA, 19081), p. 8.

Suzuki, T. (1960). Acta Crystallogr. 13, 279.

Swanson, H. E. and Tatge, E. (1953). Nat'l. Bur. Std. U.S. Circ. 539, 1, 43.

Calculated Pattern (Peak heights)

d(Å)	I	hkl	2θ(°) λ = 1.540598Å
2.7777	36	1 1 1	32.20
2.4051	100	2 0 0	37.36
1.7008	49	2 2 0	53.86
1.4504	14	3 1 1	64.16
1.3887	13	2 2 2	67.38
1.2026	5	4 0 0	79.66
1.1037	5	3 3 1	88.52
1.0757	14	4 2 0	91.46
.9820	11	4 2 2	103.34
.9259	5	5 1 1+	112.60
.8504	4	4 4 0	129.86
.8132	7	5 3 1	142.62
.8018	11	4 4 2+	147.78

Calculated Pattern (Integrated)

d(Å)	I	hkl	2θ(°) λ = 1.540598Å
2.7775	36	1 1 1	32.20
2.4054	100	2 0 0	37.35
1.7009	54	2 2 0	53.86
1.4505	16	3 1 1	64.15
1.3888	15	2 2 2	67.38
1.2027	6	4 0 0	79.65
1.1037	6	3 3 1	88.52
1.0757	17	4 2 0	91.46
.9820	14	4 2 2	103.33
.9258	5	5 1 1	112.61
.9258	2	3 3 3	112.61
.8504	8	4 4 0	129.85
.8132	16	5 3 1	142.62
.8018	22	4 4 2	147.77
.8018	6	6 0 0	147.77

Cerium zinc, CeZn₃

Structure

Orthorhombic, Amma (63), Z = 4, from powder data. The pattern is nearly identical to that of PrZn₃ (space group Pnma) except that for CeZn₃, all hkl reflections having k+l = 2n+1 were absent, suggesting a change to the A-centered lattice [Bruzzone et al., 1970].

Atom positions

The structure was determined with all atoms in positions 4(c) of Pnma.

Lattice constants

a = 6.644 Å
b = 4.627
c = 10.437
[Bruzzone et al., 1970]

CD cell: a = 6.644, b = 10.437, c = 4.627, space group Amam. a/b = 0.6366, c/b = 0.4433.

Volume Å³
320.9

Density

(calculated) 6.961 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Ce⁰, Zn⁰ [Cromer and Mann, 1968]

Scale factor (integrated intensities)

γ = 0.512 × 10⁻³

References

Bruzzone, G., Fornasini, M.L. and Merlo, F. (1970). J. Less-Common Metals 22, 253.
Cromer, D. H. and Mann, J. B. (1968). Acta Crystallogr. A24, 361.

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
4.227	5	0 1 1	21.00	
4.103	5	1 0 2	21.64	
3.567	10	1 1 1	24.94	
3.321	10	2 0 0	26.82	
2.611	100	2 1 1+	34.32	
2.564	65	1 1 3	34.96	
2.429	15	1 0 4	36.98	
2.313	35	0 2 0	38.90	
2.132	30	2 1 3	42.36	
2.039	15	3 0 2	44.40	
2.015	1	1 2 2	44.94	
1.962	5	3 1 1	46.24	
1.898	5	2 2 0	47.88	
1.731	15	0 2 4	52.84	
1.689	5	3 0 4	54.28	
1.684	5	1 0 6	54.44	
1.675	10	1 2 4	54.76	
1.661	5	4 0 0	55.26	
1.651	10	2 1 5	55.62	
1.546	5	4 1 1	59.76	
1.530	10	3 2 2	60.48	
1.4432	1	3 1 5	64.52	
1.4258	1	4 1 3	65.40	
1.4193	1	0 1 7	65.74	
1.4012	1	4 0 4	66.70	
1.3872	15	1 1 7+	67.46	
1.3793	5	1 3 3	67.90	
1.3680	5	3 0 6	68.54	
1.3641	5	3 2 4	68.76	
1.3607	5	1 2 6	68.96	
1.3494	5	4 2 0	69.62	
1.2978	5	2 3 3	72.82	
1.2803	1	1 0 8	73.98	
1.2677	1	5 1 1	74.84	
1.2144	1	2 0 8	78.74	
1.1989	10	5 1 3+	79.96	
1.1841	1	5 0 4	81.16	
1.1774	5	3 2 6	81.72	
1.1620	1	2 3 5	83.04	
1.1568	1	0 4 0	83.50	
1.1238	1	4 3 1+	86.54	
1.1203	1	1 2 8	86.88	
1.1073	1	6 0 0	88.16	
1.0752	1	2 2 8+	91.52	
1.0721	1	0 3 7+	91.86	
1.0655	1	2 1 9	92.60	
1.0583	5	1 3 7+	93.42	
1.0443	1	1 4 4+	95.06	
1.0193	1	6 0 4	98.18	
1.0111	1	3 2 8	99.26	

Cerium zinc, CeZn₃ - (Continued)

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
1.0061	1	3 4 2	99.92	
1.0020	1	5 3 1	100.48	
.9989	1	6 2 0	100.92	
.9963	1	2 0 10	101.28	
.9699	5	5 1 7	105.16	
.9671	5	5 3 3	105.60	
.9543	1	3 4 4	107.64	
.9514	1	0 2 10	108.12	
.9491	1	4 4 0	108.50	
.9338	1	7 0 2+	111.16	
.9328	1	6 2 4	111.34	
.9295	1	0 1 11	111.94	
.9146	1	2 2 10	114.76	
.8951	1	2 1 11	118.76	
.8928	1	2 3 9	119.26	
.8921	1	4 4 4+	119.42	
.8882	1	2 5 1	120.28	
.8863	1	1 5 3	120.72	
.8833	5	3 4 6+	121.40	
.8741	1	3 2 10	123.58	
.8659	1	7 2 2+	125.64	
.8636	1	2 5 3+	126.24	
.8343	5	5 3 7	134.82	
.8332	1	7 0 6+	135.20	
.8323	1	7 2 4	135.50	
.8255	1	4 2 10	137.84	
.8198	1	2 5 5	139.96	
.8149	1	8 1 1	141.90	
.8111	1	4 1 11	143.50	
.8092	1	3 0 12+	144.34	
.8081	1	0 3 11+	144.80	
.8061	1	3 4 8+	145.72	
.7999	1	6 4 0	148.72	
.7958	1	8 1 3	150.94	
.7889	1	7 1 7	155.06	
.7874	1	7 3 3+	156.10	
.7854	1	2 3 11+	157.50	
.7839	1	7 2 6	158.62	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
4.230	5	0 1 1	20.98	
4.104	5	1 0 2	21.64	
3.568	10	1 1 1	24.93	
3.322	10	2 0 0	26.82	
2.613	100	2 1 1	34.30	
2.609	30	0 0 4	34.34	
2.565	80	1 1 3	34.95	
2.429	20	1 0 4	36.98	
2.313	45	0 2 0	38.90	
2.132	35	2 1 3	42.35	
2.039	20	3 0 2	44.40	
2.015	1	1 2 2	44.94	
1.962	5	3 1 1	46.23	
1.903	1	0 1 5	47.76	
1.898	5	2 2 0	47.88	
1.739	1	0 0 6	52.57	
1.732	1	3 1 3	52.80	
1.731	15	0 2 4	52.85	
1.688	5	3 0 4	54.29	
1.683	1	1 0 6	54.48	
1.675	10	1 2 4	54.75	
1.661	5	4 0 0	55.26	
1.651	10	2 1 5	55.62	
1.546	5	4 1 1	59.77	
1.530	15	3 2 2	60.48	
1.4871	1	1 3 1	62.40	
1.4432	1	3 1 5	64.52	
1.4260	1	4 1 3	65.39	
1.4191	5	0 1 7	65.75	
1.4012	1	4 0 4	66.70	
1.3903	1	0 2 6	67.29	
1.3878	15	1 1 7	67.43	
1.3865	10	2 3 1	67.50	
1.3793	10	1 3 3	67.90	
1.3680	5	3 0 6	68.54	
1.3639	5	3 2 4	68.78	
1.3609	1	1 2 6	68.95	
1.3493	5	4 2 0	69.63	
1.2979	5	2 3 3	72.81	
1.2802	1	1 0 8	73.99	
1.2677	1	5 1 1	74.84	
1.2143	1	2 0 8	78.74	
1.1989	10	5 1 3	79.95	
1.1985	1	4 2 4	79.99	
1.1949	1	3 1 7	80.28	
1.1841	1	5 0 4	81.16	
1.1775	10	3 2 6	81.71	
1.1621	5	2 3 5	83.04	
1.1567	5	0 4 0	83.51	
1.1241	1	3 0 8	86.51	

Cerium zinc, CeZn₃ - (Continued)

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å
1.1237	1	4 3 1	86.56	
1.1201	1	1 2 8	86.90	
1.1073	1	6 0 0	88.16	
1.0823	1	3 3 5	90.76	
1.0790	1	4 1 7	91.11	
1.0752	1	2 2 8	91.52	
1.0749	1	4 3 3	91.55	
1.0720	1	0 3 7	91.87	
1.0712	1	6 1 1	91.96	
1.0655	5	2 1 9	92.60	
1.0583	5	1 3 7	93.42	
1.0575	5	0 4 4	93.51	
1.0541	1	5 2 4	93.91	
1.0443	1	1 4 4	95.05	
1.0437	1	0 0 10	95.13	
1.0193	1	6 0 4	98.17	
1.0111	1	3 2 8	99.26	
1.0061	5	3 4 2	99.93	
1.0021	1	5 3 1	100.48	
.9988	5	6 2 0	100.93	
.9957	1	2 0 10	101.36	
.9700	5	5 1 7	105.15	
.9670	5	5 3 3	105.61	
.9543	1	3 4 4	107.65	
.9514	1	0 2 10	108.13	
.9492	1	4 4 0	108.48	
.9441	1	3 0 10	109.35	
.9338	1	7 0 2	111.15	
.9328	1	6 2 4	111.34	
.9295	1	0 1 11	111.94	
.9146	1	2 2 10	114.75	
.8951	1	2 1 11	118.76	
.8928	1	2 3 9	119.26	
.8920	1	4 4 4	119.43	
.8920	1	7 0 4	119.45	
.8882	5	2 5 1	120.28	
.8863	5	1 5 3	120.71	
.8837	1	4 0 10	121.30	
.8833	5	3 4 6	121.40	
.8741	1	3 2 10	123.58	
.8730	1	6 1 7	123.85	
.8659	1	7 2 2	125.63	
.8636	1	2 5 3	126.25	
.8583	1	1 4 8	127.66	
.8376	1	2 4 8	133.76	
.8343	5	5 3 7	134.81	
.8332	1	7 0 6	135.19	
.8322	1	7 2 4	135.51	
.8274	1	5 4 4	137.16	
.8255	5	4 2 10	137.84	

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å
.8198	1	2 5 5	139.97	
.8149	5	8 1 1	141.90	
.8111	5	4 1 11	143.49	
.8081	1	0 3 11	144.79	
.8061	1	3 4 8	145.70	
.8060	1	4 5 1	145.77	
.8022	1	1 3 11	147.56	
.7999	5	6 4 0	148.73	
.7958	5	8 1 3	150.93	
.7907	1	2 2 12	153.90	
.7903	1	3 5 5	154.17	
.7890	1	7 1 7	155.03	
.7874	1	4 5 3	156.06	
.7874	1	7 3 3	156.10	
.7863	1	0 5 7	156.87	
.7855	1	1 1 13	157.43	
.7852	1	2 3 11	157.61	
.7839	5	7 2 6	158.63	

Cerium zinc, CeZn_5

Structure

Hexagonal, $P6/mmm$ (191), $Z = 1$, isostructural with CaCu_5 , from powder data [Lott and Chiotti, 1966].

Atom positions [ibid.]

1(a) 1 cerium
2(c) 2 zinc
3(g) 3 zinc

Lattice constants

A composition range exists from 70.00 to 71.97 wt.% of zinc, and the constants vary accordingly. For 70 wt.% Zn:

$a = 5.4166 \text{ \AA}$
 $c = 4.2649$

(published values: $a = 5.4163$, $c = 4.2647 \text{ \AA}$ [ibid., Table 1])

Volume \AA^3
108.4

Density
(calculated) 7.156 g/cm^3

Thermal parameters
Isotropic: overall $B = 1.0$

Scattering factors
 Ce^0 , Zn^0 [Cromer and Mann, 1968], corrected for anomalous dispersion [Cromer and Liberman, 1970].

Scale factors (integrated intensities)
 $\gamma = 0.786 \times 10^{-3}$

Additional patterns
1. Green [1973]
2. Lott and Chiotti [1966]

References

Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Green, M. L. (1973). J. Less-Common Metals 32, 391.
Lott, B. G. and Chiotti, P. (1966). Acta Crystallogr. 20, 733.

Calculated Pattern (Peak heights)

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.540598\text{\AA}$
4.69	2	1 0 0	18.92
4.26	4	0 0 1	20.82
3.16	45	1 0 1	28.26
2.707	30	1 1 0	33.06
2.345	35	2 0 0	38.36
2.286	100	1 1 1	39.38
2.132	25	0 0 2	42.36
2.055	12	2 0 1	44.02
1.676	11	1 1 2	54.74
1.637	9	2 1 1	56.14
1.578	16	2 0 2	58.44
1.564	5	3 0 0	59.02
1.468	18	3 0 1	63.30
1.360	3	1 0 3	68.98
1.354	12	2 2 0	69.34
1.261	5	3 0 2	75.32
1.259	10	1 1 3	75.46
1.245	3	3 1 1	76.48
1.216	1	2 0 3	78.64
1.173	2	4 0 0	82.12
1.143	11	2 2 2	84.72
1.131	1	4 0 1	85.88
1.109	2	2 1 3	87.98
1.066	1	0 0 4	92.52
1.052	4	3 0 3	94.16
1.043	2	3 2 1	95.16
1.028	3	4 0 2	97.12
1.024	2	4 1 0	97.62
.995	7	4 1 1	101.40
.993	4	1 1 4	101.76
.971	2	2 0 4	105.04
.960	1	3 1 3	106.76
.923	2	4 1 2	113.18
.887	2	4 2 0	120.66
.883	3	3 3 1	121.42
.881	3	3 0 4	121.94
.858	1	3 2 3	127.72
.839	1	1 0 5	133.24
.838	5	2 2 4	133.72
.831	5	4 1 3	136.04
.827	1	5 1 1	137.48
.819	3	4 2 2	140.44
.814	2	1 1 5	142.46
.789	2	4 0 4	155.06

Cerium zinc, CeZn₅ - (continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
4.69	2	1 0 0	18.90	
4.26	4	0 0 1	20.81	
3.16	40	1 0 1	28.26	
2.708	30	1 1 0	33.05	
2.345	35	2 0 0	38.35	
2.286	100	1 1 1	39.38	
2.132	25	0 0 2	42.35	
2.055	12	2 0 1	44.03	
1.675	12	1 1 2	54.74	
1.637	10	2 1 1	56.13	
1.578	17	2 0 2	58.45	
1.564	5	3 0 0	59.03	
1.468	20	3 0 1	63.30	
1.361	3	1 0 3	68.97	
1.354	14	2 2 0	69.34	
1.261	4	3 0 2	75.31	
1.259	11	1 1 3	75.46	
1.244	4	3 1 1	76.49	
1.216	1	2 0 3	78.63	
1.173	3	4 0 0	82.12	
1.143	14	2 2 2	84.73	
1.131	1	4 0 1	85.88	
1.109	2	2 1 3	87.98	
1.066	2	0 0 4	92.52	
1.052	6	3 0 3	94.16	
1.043	2	3 2 1	95.16	
1.028	3	4 0 2	97.11	
1.024	2	4 1 0	97.62	
.995	10	4 1 1	101.41	
.992	2	1 1 4	101.87	
.971	3	2 0 4	105.05	
.960	2	3 1 3	106.75	
.923	3	4 1 2	113.17	
.916	1	5 0 1	114.43	
.903	1	3 3 0	117.14	
.886	3	4 2 0	120.67	
.883	4	3 3 1	121.42	
.881	2	3 0 4	121.96	
.868	1	4 2 1	125.12	
.858	2	3 2 3	127.72	
.839	1	1 0 5	133.24	
.838	9	2 2 4	133.71	
.831	2	3 3 2	135.81	
.831	10	4 1 3	136.03	
.827	2	5 1 1	137.48	
.819	7	4 2 2	140.45	
.814	5	1 1 5	142.45	
.789	5	4 0 4	155.06	
.783	2	5 0 3	159.30	

Cerium zinc, $\text{Ce}_2\text{Zn}_{17}$

Structure

Hexagonal, $R\bar{3}m$ (166), $Z = 3$, isostructural with rhombohedral modification of U_2Zn_{17} , from powder data and qualitative single crystal analysis [Lott and Chiotti, 1966].

Atom positions

The structures of several analogous compounds have been refined and the atomic parameters are very similar [Johnson et al., 1969]. The parameters for $\text{Ce}_2\text{Zn}_{17}$ were not available, but the ratios of the cell edges c/a and of the atomic radii $r_{\text{Ce}}/r_{\text{Zn}}$ are close to the corresponding ratios for $\text{Nb}_2\text{Be}_{17}$ for which there is refined structure data [Zalkin et al., 1959]. The atomic positions for $\text{Nb}_2\text{Be}_{17}$ were used here for $\text{Ce}_2\text{Zn}_{17}$.

6(c) 6 cerium 18(f) 18 zinc(F)
6(c) 6 zinc(C) 18(h) 18 zinc(H)
9(d) 9 zinc(D)

Lattice constants, [Lott and Chiotti]

$a = 9.0713(5) \text{ \AA}$
 $c = 13.2852(5)$
(published values: $a = 9.0708$, $c = 13.2844$)

Volume
 946.8 \AA^3

Density
(calculated) 7.322 g/cm^3

Thermal parameters

Isotropic: Zn(C), $B = .81$; Zn(D), $B = 1.32$; Zn(F), $B = .74$; Zn(H), $B = 1.04$ [Johnson et al., 1969].
For Ce, $B = .54$, from their values for Pr [ibid.]

Scattering factors

Ce^0 , Zn^0 [Cromer and Mann, 1968], corrected for dispersion [Cromer and Liberman, 1970].

Scale factor (integrated intensities)
 $\gamma = 0.344 \times 10^{-3}$

References

- Cromer, D.T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
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Johnson, Q., Smith, G. S. and Wood, D. H. (1969). Acta. Crystallogr. B25, 464.
Lott, B. G. and Chiotti, P. (1966). Acta. Crystallogr. 20, 733.
Zalkin, A., Sands, D.E. and Krikorian, O.H. (1959). Acta. Crystallogr. 12, 713.

Calculated Pattern (Peak heights)

d(A)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.540598\text{\AA}$
3.767	5	0 2 1	23.60
3.381	6	2 0 2	26.34
3.169	25	1 1 3	28.14
3.058	9	1 0 4	29.18
2.8970	2	2 1 1	30.84
2.7106	7	1 2 2	33.02
2.6182	40	3 0 0	34.22
2.5364	20	0 2 4	35.36
2.5185	4	0 1 5	35.62
2.2674	65	2 2 0	39.72
2.2544	100	0 3 3+	39.96
2.2140	50	0 0 6+	40.72
2.2016	17	2 0 5	40.96
2.1504	1	1 3 1	41.98
2.0180	35	2 2 3	44.88
1.9894	6	1 1 6	45.56
1.9804	6	1 2 5	45.78
1.9427	2	4 0 1	46.72
1.8835	1	0 4 2	48.28
1.8448	2	1 0 7	49.36
1.8220	2	1 3 4	50.02
1.7860	3	3 2 1	51.10
1.7392	2	2 3 2	52.58
1.7090	2	0 2 7	53.58
1.6909	6	3 0 6+	54.20
1.5989	11	4 1 3+	57.60
1.5844	20	2 2 6+	58.18
1.5291	1	5 0 2	60.50
1.5119	4	3 3 0	61.26
1.4917	5	2 3 5	62.18
1.4309	12	3 3 3	65.14
1.4204	3	0 5 4	65.68
1.4034	4	1 1 9+	66.58
1.3800	2	1 5 2	67.86
1.3555	4	2 4 4+	69.26
1.3521	3	5 0 5	69.46
1.3093	14	6 0 0	72.08
1.3064	10	3 2 7	72.26
1.2987	4	5 1 4	72.76
1.2959	4	4 2 5	72.94
1.2859	16	0 3 9+	73.60
1.2680	1	0 4 8+	74.82
1.2585	1	0 2 10+	75.48
1.2484	1	3 3 6	76.20
1.2462	2	1 5 5	76.36
1.2371	2	2 2 9	77.02
1.2102	3	2 5 3+	79.06
1.1339	5	4 4 0	85.58
1.1324	3	5 1 7	85.72
1.1269	9	0 6 6+	86.24

Cerium zinc, Ce₂Zn₁₇ - (continued)

Calculated Pattern (Peak heights)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å
1.1186	5	4 1 9+	87.04	
1.1071	3	0 0 12+	88.18	
1.0984	1	4 4 3	89.06	
1.0752	1	2 6 2+	91.52	
1.0632	1	3 5 4	92.86	
1.0562	6	3 3 9	93.66	
1.0351	2	6 2 4	96.18	
1.0339	1	5 3 5	96.32	
1.0197	2	3 0 12+	98.12	
1.0130	3	7 1 3+	99.00	
1.0093	4	4 4 6	99.50	
1.0081	2	2 6 5	99.66	
.9949	3	2 2 12	101.48	
.9898	1	6 3 0+	102.20	
.9660	5	6 3 3+	105.76	
.9574	2	2 5 9+	107.14	
.9449	1	6 2 7	109.22	
.9416	1	0 8 4	109.78	
.9407	1	4 5 5	109.94	
.9220	1	2 7 4	113.32	
.8932	1	3 3 12	119.18	
.8888	3	3 2 13+	120.14	
.8863	2	8 1 4	120.72	
.8821	1	3 4 11+	121.68	
.8689	1	1 8 5	124.88	
.8572	4	8 2 0+	127.96	
.8505	3	7 1 9+	129.84	

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å
3.767	7	0 2 1	23.60	
3.381	9	2 0 2	26.34	
3.169	40	1 1 3	28.14	
3.059	15	1 0 4	29.17	
2.8978	3	2 1 1	30.83	
2.7108	11	1 2 2	33.02	
2.6187	70	3 0 0	34.21	
2.5362	40	0 2 4	35.36	
2.5170	4	0 1 5	35.64	
2.2678	100	2 2 0	39.71	
2.2541	85	3 0 3	39.97	
2.2541	85	0 3 3	39.97	
2.2142	60	0 0 6	40.72	
2.2136	30	2 1 4	40.73	
2.2008	18	2 0 5	40.98	
2.1501	1	1 3 1	41.99	
2.0185	60	2 2 3	44.87	
1.9898	10	1 1 6	45.55	
1.9800	10	1 2 5	45.79	
1.9429	4	4 0 1	46.72	
1.8834	3	0 4 2	48.28	
1.8448	3	1 0 7	49.36	
1.8218	3	1 3 4	50.03	
1.7859	6	3 2 1	51.10	
1.7394	5	2 3 2	52.57	
1.7143	1	4 1 0	53.40	
1.7089	3	0 2 7	53.59	
1.6908	6	3 0 6	54.21	
1.6908	5	0 3 6	54.21	
1.6848	1	3 1 5	54.41	
1.5991	7	2 1 7	57.59	
1.5987	8	4 1 3	57.61	
1.5987	7	1 4 3	57.61	
1.5843	25	2 2 6	58.18	
1.5841	12	3 2 4	58.19	
1.5603	1	0 5 1	59.17	
1.5290	2	5 0 2	60.50	
1.5119	7	3 3 0	61.26	
1.4915	9	2 3 5	62.19	
1.4311	1	1 3 7	65.13	
1.4308	25	3 3 3	65.15	
1.4203	5	0 5 4	65.69	
1.4037	7	1 1 9	66.57	
1.4031	2	5 1 1	66.60	
1.3802	3	1 5 2	67.85	
1.3555	1	4 1 6	69.26	
1.3555	1	1 4 6	69.26	
1.3554	6	2 4 4	69.27	
1.3524	2	5 0 5	69.44	
1.3093	25	6 0 0	72.08	

Cerium zinc, Ce₂Zn₁₇ - (continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
1.3069	7	3 2 7	72.23	
1.2986	7	5 1 4	72.76	
1.2960	4	4 2 5	72.93	
1.2859	14	3 0 9	73.60	
1.2859	15	0 3 9	73.60	
1.2855	2	4 3 1	73.63	
1.2681	2	0 4 8	74.81	
1.2585	2	0 2 10	75.48	
1.2486	2	3 3 6	76.19	
1.2462	3	1 5 5	76.36	
1.2371	3	2 2 9	77.02	
1.2103	2	0 5 7	79.06	
1.2101	2	5 2 3	79.07	
1.2101	3	2 5 3	79.07	
1.1694	1	2 4 7	82.41	
1.1339	11	4 4 0	85.58	
1.1323	4	5 1 7	85.73	
1.1270	9	6 0 6	86.23	
1.1270	9	0 6 6	86.23	
1.1186	4	4 1 9	87.04	
1.1186	4	1 4 9	87.04	
1.1183	1	3 5 1	87.07	
1.1071	5	0 0 12	88.18	
1.1066	1	5 3 2	88.23	
1.1066	1	0 7 2	88.23	
1.0985	2	4 4 3	89.05	
1.0858	1	6 2 1	90.38	
1.0751	1	2 6 2	91.53	
1.0632	3	3 5 4	92.85	
1.0563	1	3 1 11	93.64	
1.0562	11	3 3 9	93.66	
1.0405	1	7 1 0	95.51	
1.0352	5	6 2 4	96.17	
1.0338	2	5 3 5	96.33	
1.0197	1	0 3 12	98.12	
1.0197	2	3 0 12	98.12	
1.0134	1	1 0 13	98.95	
1.0130	3	7 1 3	99.01	
1.0130	3	1 7 3	99.01	
1.0093	8	4 4 6	99.50	
1.0080	3	2 6 5	99.67	
1.0030	1	5 4 1	100.35	
.9949	6	2 2 12	101.48	
.9900	1	2 4 10	102.17	
.9898	2	6 3 0	102.20	
.9672	1	5 1 10	105.57	
.9663	3	2 1 13	105.72	
.9660	2	3 5 7	105.76	
.9659	4	6 3 3	105.78	
.9659	4	3 6 3	105.78	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
.9627	2	5 4 4	106.29	
.9575	3	5 2 9	107.13	
.9575	3	2 5 9	107.13	
.9448	2	6 2 7	109.23	
.9417	1	0 8 4	109.77	
.9407	2	4 5 5	109.94	
.9299	1	0 7 8	111.87	
.9252	1	1 3 13	112.72	
.9220	2	2 7 4	113.32	
.9211	1	8 0 5	113.50	
.9173	1	8 1 1	114.23	
.9108	1	1 8 2	115.50	
.8932	2	3 3 12	119.17	
.8890	4	3 2 13	120.11	
.8888	3	5 4 7	120.16	
.8887	1	5 5 3	120.18	
.8861	4	8 1 4	120.75	
.8821	2	3 4 11	121.67	
.8819	1	7 3 1	121.72	
.8689	2	1 8 5	124.87	
.8572	11	8 2 0	127.97	
.8567	2	0 5 13	128.10	
.8565	1	2 7 7	128.15	
.8564	1	9 0 3	128.17	
.8564	2	0 9 3	128.17	
.8505	5	7 1 9	129.84	
.8505	4	1 7 9	129.84	

Cesium cerium chloride, Cs₂CeCl₆

Structure

Hexagonal, P $\bar{3}$ m1 (164), Z=1 [Kaatz and Marcovich, 1966].

Atom positions

1(a) 1 cerium
2(d) 2 cesium
6(l) 6 chlorine

Lattice constants [ibid.]

a = 7.476(2) Å
c = 6.039(2)

c/a = 0.8078

Volume

292.3 Å³

Density

(calculated) 3.52 g/cm³
[Kaatz and Marcovich, 1966].

Thermal parameters

Isotropic [Kaatz and Marcovich, 1966].

Scattering factors

Cl⁻ [Dawson, 1960]
Cs⁺, Ce⁴⁺ [Thomas and Umeda, 1957]

Scale factors (integrated intensities)

$\gamma = 0.648 \times 10^{-3}$

References

Dawson, B. (1960). Acta Crystallogr. 13, 403.
Kaatz, T. and Marcovich, M. (1966). Acta Crystallogr. 21, 1011.
Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 6, 293.

Calculated Pattern (Peak heights)			
d(Å)	I	hkl	2 θ (°) $\lambda = 1.540598\text{Å}$
6.47	2	100	13.68
6.04	4	001	14.66
4.41	100	011	20.10
3.74	29	110	23.80
3.24	2	200	27.54
3.18	6	111	28.06
3.02	6	002	29.56
2.852	6	201+	31.34
2.736	12	102+	32.70
2.267	22	121	39.72
2.208	14	202+	40.84
2.158	5	300	41.82
2.032	1	301+	44.56
1.922	6	103	47.26
1.901	6	212+	47.80
1.869	10	220	48.68
1.772	1	113	51.52
1.721	8	311	53.18
1.710	1	023	53.56
1.589	3	222	57.98
1.563	1	041+	59.04
1.555	4	213	59.40
1.543	3	132+	59.88
1.510	1	004	61.36
1.442	4	231+	64.56
1.427	2	042+	65.36
1.413	2	410	66.08
1.400	2	114	66.78
1.340	2	133+	70.18
1.333	2	322+	70.62
1.266	1	501	74.94
1.237	1	304+	77.02
1.195	1	323+	80.26
1.187	1	015	80.90
1.174	2	224	81.98
1.142	1	151	84.84
1.134	1	422+	85.58
1.083	1	125	90.68
1.079	1	600	91.10
1.032	1	144+	96.62
1.002	1	315	100.46
0.9143	1	531+	114.82
.8779	1	064+	122.66

Cesium cerium chloride, Cs₂CeCl₆ - (continued)

Calculated Pattern (Integrated)			
d(Å)	I	hkl	2θ(°) λ = 1.540598Å
6.47	2	100	13.67
6.04	4	001	14.66
4.42	14	101	20.09
4.42	100	011	20.09
3.74	34	110	23.78
3.24	3	200	27.53
3.18	8	111	28.05
3.02	8	002	29.56
2.853	5	201	31.33
2.853	2	021	31.33
2.737	6	012	32.70
2.737	9	102	32.70
2.268	3	211	39.71
2.268	26	121	39.71
2.208	10	202	40.83
2.208	9	022	40.83
2.158	7	300	41.82
2.032	1	301	44.55
1.922	7	103	47.25
1.922	7	013	47.25
1.901	5	212	47.80
1.901	3	122	47.80
1.869	13	220	48.68
1.785	1	221	51.12
1.772	1	113	51.52
1.721	10	311	53.17
1.721	1	131	53.17
1.709	1	023	53.57
1.599	4	222	57.99
1.563	1	041	59.04
1.555	6	213	59.41
1.543	2	312	59.88
1.543	2	132	59.88
1.510	2	004	61.36
1.442	5	231	64.56

Calculated Pattern (Integrated)			
d(Å)	I	hkl	2θ(°) λ = 1.540598Å
1.427	2	042	65.36
1.427	2	402	65.36
1.413	3	410	66.08
1.400	2	114	66.77
1.370	1	223	68.44
1.340	3	133	70.18
1.333	1	322	70.61
1.333	1	232	70.61
1.266	1	501	74.95
1.246	1	330	76.37
1.237	1	304	77.02
1.195	2	323	80.26
1.187	1	015	80.90
1.174	3	224	81.97
1.142	1	151	84.85
1.134	1	422	85.58
1.134	1	242	85.58
1.083	1	125	90.67
1.079	1	600	91.10
1.048	1	341	94.59
1.007	1	513	99.82
1.002	1	315	100.46
0.9744	1	611	104.47
.9409	1	433	109.90
.9371	1	235	110.57
.9345	1	440	111.03
.9143	1	531	114.82
.8865	1	163	120.68
.8377	1	155	133.72
.8213	1	451	139.42
.8136	1	217	142.43
.7985	1	345	149.43
.7946	2	444	151.59
.7843	1	721	158.33

Chlorpromazine, C₁₇H₁₉ClN₂S

Synonym

3-chloro-10-(3'-dimethylamino-n-propyl)-pheno-thiazine

Stability

The material was unstable in light, air, and x-rays [McDowell, 1969].

Structure

Orthorhombic, Pbca (61), Z = 8. The structure was determined by McDowell [ibid.].

Atom positions

All the atoms were in general positions [ibid.].

Lattice constants [ibid.]

a = 23.50(4) Å

b = 15.20(2)

c = 9.23(1)

CD cell: a = 15.20, b = 23.50, c = 9.23, space group Pcab; a/b = 0.6468, c/b = 0.3928

Volume

3297. Å³

Density

(measured) 1.289 g/cm³

(calculated) 1.285 g/cm³

Thermal parameters

Isotropic: overall B = 5.0

Scattering factors

C⁰, Cl⁰, N⁰, S⁰ [International Tables, 1962]

Scale factors (integrated intensities)

$\gamma = 0.545 \times 10^{-3}$

I/I_c (calculated) = 0.88

References

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.), p. 202.

McDowell, J. J. H. (1969). Acta Crystallogr. B25 2175.

Calculated Pattern (Peak heights)					
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å	
4.04	6	5 1 1	22.00		
3.97	36	3 0 2	22.36		
3.89	22	1 2 2	22.86		
3.84	9	4 3 0+	23.16		
3.79	4	6 1 0+	23.44		
3.74	4	2 2 2	23.78		
3.67	5	5 2 1	24.26		
3.63	5	4 0 2	24.52		
3.52	16	3 2 2+	25.26		
3.47	8	1 4 1	25.62		
3.38	11	1 3 2	26.38		
3.27	11	4 2 2	27.22		
3.20	5	3 4 1	27.82		
3.13	6	3 3 2	28.52		
3.09	2	7 1 1+	28.86		
3.02	2	5 2 2	29.54		
2.990	2	1 1 3	29.86		
2.934	3	8 0 0+	30.44		
2.845	1	2 4 2	31.42		
2.813	2	3 1 3	31.78		
2.748	3	8 1 1+	32.56		
2.701	4	4 5 0+	33.14		
2.677	6	7 3 1+	33.44		
2.614	3	1 3 3	34.28		
2.592	2	4 5 1	34.58		
2.556	1	7 2 2	35.08		
2.538	1	5 1 3+	35.34		
2.524	1	1 5 2	35.54		
2.493	2	3 3 3	36.00		
2.477	2	2 6 0+	36.24		
2.400	1	4 3 3	37.44		
2.393	1	0 4 3	37.56		
2.355	1	8 2 2	38.18		
2.342	2	2 4 3	38.40		
2.332	3	3 6 1	38.58		
2.295	1	5 3 3+	39.22		
2.264	1	2 0 4	39.78		
2.255	1	4 6 1+	39.94		
2.244	1	7 1 3+	40.16		
2.234	1	5 5 2	40.34		
2.227	1	8 3 2	40.48		
2.214	2	4 4 3	40.72		
2.209	3	7 4 2+	40.82		
2.177	2	9 2 2+	41.44		
2.130	3	6 5 2+	42.40		
2.127	3	6 6 0+	42.46		
2.105	2	8 1 3+	42.94		
2.084	1	3 5 3	43.38		
2.067	4	4 2 4+	43.76		
2.040	1	6 4 3	44.36		
2.037	1	4 7 0	44.44		

Calculated Pattern (Peak heights)					
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å	
11.75	100	2 0 0	7.52		
9.28	2	2 1 0	9.52		
7.60	13	0 2 0	11.64		
7.48	10	1 1 1	11.82		
6.54	5	2 1 1	13.52		
6.38	1	2 2 0	13.88		
5.86	36	0 2 1	15.10		
5.69	7	1 2 1	15.56		
5.47	7	4 1 0	16.18		
5.25	35	2 2 1	16.88		
4.69	4	3 2 1	18.92		
4.61	41	0 0 2	19.22		
4.36	19	1 3 1	20.34		
4.30	5	2 0 2	20.66		
4.15	75	2 3 1	21.38		

Chlorpromazine, C₁₇H₁₉ClN₂S - (Continued)

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598Å
11.75	100	2 0 0	7.52	
9.30	2	2 1 0	9.51	
7.60	13	0 2 0	11.63	
7.48	9	1 1 1	11.82	
6.55	5	2 1 1	13.51	
6.38	1	2 2 0	13.87	
5.87	2	4 0 0	15.07	
5.87	36	0 2 1	15.09	
5.69	6	1 2 1	15.55	
5.48	7	4 1 0	16.16	
5.25	38	2 2 1	16.88	
4.70	2	3 2 1	18.88	
4.65	1	4 2 0	19.08	
4.62	45	0 0 2	19.22	
4.36	20	1 3 1	20.33	
4.34	2	1 1 2	20.45	
4.30	4	2 0 2	20.66	
4.15	81	2 3 1	21.37	
4.15	2	4 2 1	21.39	
4.13	4	2 1 2	21.48	
4.04	4	5 1 1	22.00	
3.98	40	3 0 2	22.34	
3.94	4	0 2 2	22.52	
3.89	23	1 2 2	22.84	
3.86	1	3 3 1	23.00	
3.85	2	3 1 2	23.10	
3.84	7	4 3 0	23.16	
3.80	1	0 4 0	23.39	
3.79	3	6 1 0	23.44	
3.74	4	2 2 2	23.77	
3.67	5	5 2 1	24.24	
3.63	6	4 0 2	24.51	
3.54	5	4 3 1	25.11	
3.53	3	4 1 2	25.21	
3.52	14	3 2 2	25.26	
3.51	3	0 4 1	25.33	
3.51	2	6 1 1	25.37	
3.48	1	6 2 0	25.57	
3.48	7	1 4 1	25.61	
3.38	12	1 3 2	26.38	
3.37	2	2 4 1	26.45	
3.29	4	5 0 2	27.06	
3.27	11	4 2 2	27.21	
3.21	5	3 4 1	27.80	
3.19	4	4 4 0	27.94	
3.13	7	3 3 2	28.51	
3.10	1	6 3 0	28.79	
3.09	1	7 1 1	28.88	
3.02	2	5 2 2	29.54	
2.991	2	1 1 3	29.85	

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598Å
2.950	1	4 3 2	30.27	
2.937	2	8 0 0	30.40	
2.934	1	0 4 2	30.45	
2.930	1	6 1 2	30.48	
2.846	1	2 4 2	31.41	
2.814	2	3 1 3	31.77	
2.753	2	8 1 1	32.50	
2.747	1	3 4 2	32.57	
2.709	3	3 5 1	33.04	
2.700	3	4 5 0	33.15	
2.683	3	4 1 3	33.37	
2.678	4	7 3 1	33.43	
2.673	1	7 1 2	33.50	
2.625	1	4 4 2	34.14	
2.613	3	1 3 3	34.28	
2.591	2	4 5 1	34.59	
2.557	1	7 2 2	35.07	
2.538	1	5 1 3	35.34	
2.524	1	1 5 2	35.54	
2.493	3	3 3 3	36.00	
2.476	1	2 6 0	36.25	
2.400	1	4 3 3	37.44	
2.391	1	0 4 3	37.59	
2.356	1	8 2 2	38.17	
2.343	2	2 4 3	38.39	
2.332	3	3 6 1	38.57	
2.295	1	5 3 3	39.22	
2.264	1	2 0 4	39.78	
2.256	1	4 6 1	39.93	
2.243	1	7 1 3	40.16	
2.234	1	5 5 2	40.35	
2.226	1	8 3 2	40.49	
2.215	2	4 4 3	40.71	
2.209	1	7 4 2	40.82	
2.177	2	9 2 2	41.44	
2.137	1	3 6 2	42.27	
2.130	2	6 5 2	42.40	
2.127	1	6 6 0	42.46	
2.104	2	8 1 3	42.95	
2.084	1	3 5 3	43.37	
2.073	2	6 6 1	43.63	
2.070	1	7 3 3	43.69	
2.067	3	4 2 4	43.76	
2.062	2	11 1 1	43.87	
2.041	1	6 4 3	44.35	
2.037	1	4 7 0	44.44	

Chromium cobalt silicide, $\text{Co}_9\text{Cr}_{15}\text{Si}_6$

Structure

Tetragonal, $P4_2/mnm(136)$, $Z = 1$, σ -phase, iso-structural with σ -(Cr, Fe), from powder data, [Stüwe, 1959]. Much work has been done on the σ -phase structure which has multiple atoms in 5 sites, called A through E [Bergman and Shoemaker, 1954]. The ordering arrangement of the atoms is dependent on a complex combination of electronic and size factors [Spooner, 1968].

Atom positions

The positions used were those for σ -(Cr, Fe) [Spooner and Wilson, 1964], and for σ -(X, Y, Si) [Aronsson and Lundström, 1957]. Site occupancy shared by multiple atoms was assumed to be random and in the following proportions:

Site A: 2(a) 2.0 cobalt

Site B: 4(f) 4.0 chromium

Site C: 8(i) 5.5 chromium and 2.5 cobalt

Site D: 8(i) 6.0 silicon and 2 cobalt

Site E: 8(j) 5.5 chromium and 2.5 cobalt

Lattice constants [Stüwe, 1959]

$a = 8.736 \text{ \AA}$

$c = 4.561$

Volume

348.12 \AA^3

Density

(calculated) 7.054 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Scattering factors

Co^0 , Cr^0 , Si^0 [Cromer and Mann, 1968].

Scale factor (integrated intensities)

$\gamma = 0.146 \times 10^{-3}$

References

- Aronsson, B. and Lundström, T. (1957). Acta Chem. Scand. 11, 365.
 Bergman, G. and Shoemaker, D.P. (1954). Acta Crystallogr. 7, 857.
 Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
 Spooner, F. J. (1968). Acta Crystallogr. A24, 605.
 Spooner, F.J. and Wilson, C.G. (1964). Acta Crystallogr. 17, 1533.
 Stüwe, H. P. (1959). Trans. AIME 215, 408.

Calculated Pattern (Peak heights)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
3.904	4	2 1 0	22.76	
3.089	3	2 2 0	28.88	
2.967	7	2 1 1	30.10	
2.455	1	3 0 1	36.58	
2.423	2	3 2 0	37.08	
2.362	14	3 1 1	38.06	
2.281	19	0 0 2	39.48	
2.139	5	1 1 2	42.22	
2.119	90	4 1 0	42.64	
2.059	50	3 3 0	43.94	
2.021	50	2 0 2	44.80	
1.970	65	2 1 2	46.04	
1.922	100	4 1 1	47.26	
1.877	35	3 3 1	48.46	
1.834	7	2 2 2	49.66	
1.758	15	3 1 2	51.96	
1.713	1	5 1 0	53.44	
1.660	2	3 2 2	55.28	
1.632	3	4 3 1	56.34	
1.604	1	5 1 1	57.40	
1.529	1	5 2 1	60.52	
1.387	4	4 3 2	67.48	
1.370	2	5 1 2+	68.44	
1.332	1	3 1 3	70.66	
1.322	8	5 2 2+	71.28	
1.2523	15	5 3 2	75.92	
1.2352	19	4 1 3+	77.16	
1.2272	5	6 0 2	77.76	
1.2232	7	3 3 3	78.06	
1.2154	5	6 1 2	78.66	
1.2036	2	7 0 1	79.58	
1.2001	11	7 2 0	79.86	
1.1924	5	5 5 1	80.48	
1.1815	4	6 2 2	81.38	
1.1708	3	5 4 2+	82.28	
1.1604	6	7 2 1	83.18	
1.1470	1	4 3 3	84.38	
1.1402	6	0 0 4	85.00	
1.0619	1	7 2 2	93.00	
1.0595	6	8 2 0	93.28	
1.0320	4	8 2 1	96.56	
1.0295	4	6 6 0	96.88	
1.0041	10	4 1 4+	100.20	
.9976	5	3 3 4	101.10	
.9850	4	8 0 2	102.90	
.9787	7	7 4 2	103.82	
.9609	1	8 2 2	106.58	
.9587	2	5 5 3	106.92	
.9420	3	7 2 3	109.72	
.9277	1	9 2 1+	112.26	

Chromium cobalt silicide, $\text{Co}_9\text{Cr}_{15}\text{Si}_6$ - (continued)

Calculated Pattern (Peak heights)					
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å	
.8886	1	9 1 2	120.20		
.8750	3	7 6 2+	123.36		
.8692	3	8 2 3+	124.80		
.8581	1	8 5 2+	127.72		
.8539	2	9 3 2+	128.86		
.8525	2	6 6 3	129.26		
.8379	7	4 1 5+	133.66		
.8340	2	3 3 5	134.92		
.8267	9	7 2 4+	137.44		
.8231	1	10 3 1	138.74		

Calculated Pattern (Integrated)					
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å	
3.907	3	2 1 0	22.74		
3.089	2	2 2 0	28.88		
2.967	6	2 1 1	30.09		
2.455	1	3 0 1	36.58		
2.423	2	3 2 0	37.07		
2.363	13	3 1 1	38.05		
2.280	18	0 0 2	39.48		
2.139	3	1 1 2	42.21		
2.119	85	4 1 0	42.63		
2.059	45	3 3 0	43.93		
2.022	45	2 0 2	44.80		
1.970	65	2 1 2	46.05		
1.922	100	4 1 1	47.26		
1.877	35	3 3 1	48.46		
1.835	7	2 2 2	49.65		
1.759	15	3 1 2	51.95		
1.713	1	5 1 0	53.43		
1.661	2	3 2 2	55.27		
1.632	3	4 3 1	56.34		
1.604	1	5 1 1	57.40		
1.529	1	5 2 1	60.52		
1.387	4	4 3 2	67.47		
1.370	2	5 1 2	68.43		
1.364	1	5 4 0	68.74		
1.332	1	3 1 3	70.66		
1.322	2	6 2 1	71.27		
1.322	7	5 2 2	71.28		
1.2522	17	5 3 2	75.93		
1.2355	5	5 5 0	77.14		
1.2353	17	4 1 3	77.16		
1.2273	5	6 0 2	77.76		
1.2231	7	3 3 3	78.07		
1.2153	6	6 1 2	78.67		
1.2038	1	7 0 1	79.57		
1.2001	12	7 2 0	79.87		

Calculated Pattern (Integrated)					
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å	
1.1925	5	5 5 1	80.47		
1.1815	4	6 2 2	81.38		
1.1709	1	6 4 1	82.27		
1.1709	2	5 4 2	82.28		
1.1606	7	7 2 1	83.17		
1.1469	1	4 3 3	84.38		
1.1402	7	0 0 4	84.99		
1.0699	1	6 4 2	92.10		
1.0620	1	7 2 2	92.99		
1.0595	7	8 2 0	93.28		
1.0320	4	8 2 1	96.56		
1.0296	3	6 6 0	96.86		
1.0043	3	6 6 1	100.17		
1.0041	10	4 1 4	100.20		
.9975	6	3 3 4	101.10		
.9850	4	8 0 2	102.90		
.9788	8	7 4 2	103.82		
.9608	1	8 2 2	106.59		
.9588	3	5 5 3	106.91		
.9420	4	7 2 3	109.72		
.8885	1	9 1 2	120.21		
.8751	2	9 2 2	123.35		
.8751	2	7 6 2	123.35		
.8692	3	8 2 3	124.80		
.8580	1	8 5 2	127.73		
.8539	3	9 3 2	128.87		
.8525	3	6 6 3	129.26		
.8379	5	5 5 4	133.64		
.8379	8	4 1 5	133.67		
.8340	3	3 3 5	134.91		
.8267	5	9 4 2	137.42		
.8266	13	7 2 4	137.46		
.8231	2	10 3 1	138.74		
.8218	1	8 4 3	139.22		

Cobalt copper tin, CoCu_2Sn

Structure

Cubic, $\text{Fm}\bar{3}\text{m}$ (225), $Z = 4$, a Heusler alloy iso-structural with Cu_2AlMn , from powder data [Dwight 1967].

Atom positions [ibid.]

4(b) 4 cobalt
8(c) 8 copper
4(a) 4 tin

Lattice constant [ibid.]

$a = 5.982 \text{ \AA}$

Volume

214.1 \AA^3

Density

(calculated) 9.454 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Scattering factors

Co^0 , Cu^0 , Sn^0 [Cromer and Mann, 1968].

Scale factor (integrated intensities)

$\gamma = 1.42 \times 10^{-3}$

References

Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Dwight, A.E. (1967). Intermetallic Compounds (Wiley and Sons Inc., New York), Westbrook, J. H. (ed.) p. 174.

Calculated Pattern (Peak heights)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
3.453	10	1 1 1	25.78	
2.990	3	2 0 0	29.86	
2.115	100	2 2 0	42.72	
1.804	4	3 1 1	50.56	
1.496	13	4 0 0	62.00	
1.372	1	3 3 1	68.30	
1.221	20	4 2 2	78.22	
1.151	1	5 1 1+	84.00	
1.057	6	4 4 0	93.52	
1.011	1	5 3 1	99.24	
.9458	8	6 2 0	109.06	
.8635	2	4 4 4	126.28	
.7994	13	6 4 2	149.00	
.7788	1	7 3 1+	163.06	

Calculated Pattern (Integrated)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
3.454	9	1 1 1	25.77	
2.991	2	2 0 0	29.85	
2.115	100	2 2 0	42.72	
1.804	4	3 1 1	50.56	
1.495	14	4 0 0	62.01	
1.372	1	3 3 1	68.29	
1.338	1	4 2 0	70.32	
1.221	25	4 2 2	78.22	
1.151	1	5 1 1	84.00	
1.057	7	4 4 0	93.51	
1.011	1	5 3 1	99.25	
.9458	11	6 2 0	109.06	
.8634	4	4 4 4	126.29	
.7994	30	6 4 2	149.00	
.7788	1	5 5 3	163.06	
.7788	3	7 3 1	163.06	

Structure

Cubic, Fm3m (225), Z = 4, a Heusler alloy iso-structural with Cu₂AlMn, from powder data (x-ray and neutron) [Ziebeck and Webster, 1974].

Atom positions [ibid.]

8(c) 8 cobalt
4(a) 4 gallium
4(b) 4 hafnium

Lattice constant [ibid.]

a = 6.032 Å

Volume

219.5 Å³

Density

(measured) 11.10 g/cm³ [ibid.]
(calculated) 11.08 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co⁰, Ga⁰, Hf⁰ [Cromer and Mann, 1968] corrected for anomalous dispersion [Cromer and Liberman, 1970].

Scale factor (integrated intensities)

$\gamma = 1.287 \times 10^{-3}$

References

- Cromer, D.T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Ziebeck, K. R. A. and Webster, P. J. (1974). J. Phys. Chem. Solids 35, 1.

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
3.482	20	1 1 1	25.56	
3.016	18	2 0 0	29.60	
2.132	100	2 2 0	42.36	
1.819	9	3 1 1	50.12	
1.741	4	2 2 2	52.52	
1.508	13	4 0 0	61.44	
1.384	3	3 3 1	67.64	
1.349	5	4 2 0	69.66	
1.231	20	4 2 2	77.46	
1.161	2	5 1 1+	83.14	
1.066	6	4 4 0	92.50	
1.020	2	5 3 1	98.14	
1.005	2	4 4 2+	100.04	
.9537	8	6 2 0	107.74	
.9198	1	5 3 3	113.74	
.9093	1	6 2 2	115.80	
.8706	2	4 4 4	124.44	
.8446	1	5 5 1+	131.56	
.8365	1	6 4 0	134.10	
.8061	12	6 4 2	145.74	
.7853	2	7 3 1+	157.56	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
3.483	19	1 1 1	25.56	
3.016	17	2 0 0	29.60	
2.133	100	2 2 0	42.35	
1.819	9	3 1 1	50.12	
1.741	5	2 2 2	52.51	
1.508	14	4 0 0	61.44	
1.384	3	3 3 1	67.65	
1.349	6	4 2 0	69.65	
1.231	25	4 2 2	77.45	
1.161	2	5 1 1	83.14	
1.066	7	4 4 0	92.50	
1.020	2	5 3 1	98.14	
1.005	2	4 4 2	100.03	
.9537	11	6 2 0	107.74	
.9199	1	5 3 3	113.73	
.9094	2	6 2 2	115.79	
.8706	3	4 4 4	124.44	
.8446	1	7 1 1	131.56	
.8446	1	5 5 1	131.56	
.8365	2	6 4 0	134.11	
.8061	30	6 4 2	145.74	
.7853	2	5 5 3	157.57	
.7853	5	7 3 1	157.57	

Cobalt gallium niobium, Co₂GaNb

Structure

Cubic, Fm3m (225), Z = 4, a Heusler alloy iso-structural with Cu₂AlMn, from powder data [Markiv et al., 1965].

Atom positions [ibid.]

8(c) 8 cobalt
4(a) 4 gallium
4(b) 4 niobium

Lattice constant [ibid.]

a = 5.954 Å

Volume

211.1 Å³

Density

(calculated) 8.826 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co⁰, Ga⁰, Nb⁰ [Cromer and Mann, 1968]

Scale factors (integrated intensities)

γ = 1.18 × 10⁻³

References

Cromer, D. T. and Mann, J. B. (1968). Acta Cryst-allogr. A24, 321.
Markiv, V.Ya., Voroshilov, Yu.V., Kripyakevich, P.I. and Cherkashin, E.E. (1965). Sov. Phys.-Crystal-logr. 9, 619.

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
3.437	2	1 1 1	25.90	
2.976	4	2 0 0	30.00	
2.105	100	2 2 0	42.94	
1.719	1	2 2 2	53.26	
1.488	13	4 0 0	62.34	
1.331	1	4 2 0	70.70	
1.2154	20	4 2 2	78.66	
1.0526	6	4 4 0	94.08	
.9414	9	6 2 0	109.82	
.8594	2	4 4 4	127.36	
.7956	14	6 4 2	151.00	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
3.438	2	1 1 1	25.90	
2.977	3	2 0 0	29.99	
2.105	100	2 2 0	42.93	
1.719	1	2 2 2	53.25	
1.488	14	4 0 0	62.33	
1.331	1	4 2 0	70.70	
1.2154	25	4 2 2	78.66	
1.0525	7	4 4 0	94.08	
.9414	12	6 2 0	109.82	
.8594	4	4 4 4	127.36	
.7956	35	6 4 2	151.00	

Cobalt germanium, Co_3Ge_2

Structure

Hexagonal, $P6_3/mmc$ (194), $Z = 1$, isostructural with Ni_2In and Ni_3Sn_2 , from powder data [Lecocq and Michel, 1964].

Atom positions

The structure prototype, $2(\text{Ni}_2\text{In})$, has 2 Ni atoms in positions 2(a) and also in 2(d); the indium are in 2(c). Studies on two isostructural compounds, Ni_3In_2 and Co_3Sn_2 , indicated that in their structures the site 2(d) is only partially occupied [Kanematsu, 1962; Rajeswari and Manohar, 1970].

The positions used here for Co_3Ge_2 were:

2(a) 2 cobalt
2(d) 1 cobalt
2(c) 2 germanium

Lattice constants [Lecocq and Michel, 1964]

A composition range exists from 36 to 44 atomic percent Ge and the constants vary accordingly. For 40 atomic percent Ge:

$a = 3.964 \text{ \AA}$
 $c = 4.992$

Volume

67.93 \AA^3

Density

(calculated) 7.870 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Scattering factors

Co^0 , Ge^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)

$\gamma = 0.418 \times 10^{-3}$

References

- Cromer, D. T. and Mann, J. B. (1968) Acta Crystallogr. **A24**, 321.
Kanematsu, K. (1962). J. Phys. Soc. Jap. **17**, 85.
Lecocq, P. and Michel, A. (1964). Bull. Soc. Chim. Fr. **1964**, 1911.
Rajeswari, H. and Manohar, H. (1970). Indian J. Pure Appl. Phys. **8**, 363.

Calculated Pattern (Peak heights)

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.540598\text{\AA}$
3.432	2	1 0 0	25.94
2.827	35	1 0 1	31.62
2.495	5	0 0 2	35.96
2.019	100	1 0 2	44.86
1.982	100	1 1 0	45.74
1.623	5	2 0 1	56.66
1.552	6	1 1 2	59.50
1.497	4	1 0 3	61.92
1.414	25	2 0 2	66.00
1.256	4	2 1 1	75.68
1.248	5	0 0 4	76.22
1.195	1	2 0 3	80.30
1.151	19	2 1 2	84.00
1.144	10	3 0 0	84.62
1.056	15	1 1 4	93.68
1.040	1	3 0 2	95.56
1.023	2	2 1 3	97.68
.991	6	2 2 0	102.02
.935	1	3 1 1	110.90
.921	1	2 2 2	113.50
.890	8	3 1 2	119.98
.843	8	3 0 4	131.92
.826	1	3 1 3	137.54
.812	3	4 0 2	143.28
.809	4	1 0 6	144.60
.7913	1	2 1 5	153.56
.7779	1	3 2 1	163.92

Cobalt germanium, Co_3Ge_2 - (continued)

Calculated Pattern (Integrated)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
3.433	2	1 0 0	25.93	
2.829	30	1 0 1	31.61	
2.496	5	0 0 2	35.95	
2.019	100	1 0 2	44.86	
1.982	100	1 1 0	45.74	
1.623	5	2 0 1	56.66	
1.552	6	1 1 2	59.51	
1.497	4	1 0 3	61.92	
1.414	25	2 0 2	66.00	
1.256	4	2 1 1	75.67	
1.248	5	0 0 4	76.23	
1.195	2	2 0 3	80.29	
1.151	20	2 1 2	83.99	
1.144	12	3 0 0	84.62	
1.056	18	1 1 4	93.67	
1.040	1	3 0 2	95.55	
1.023	2	2 1 3	97.67	
.991	7	2 2 0	102.03	
.959	1	1 0 5	106.93	
.935	2	3 1 1	110.90	
.921	1	2 2 2	113.51	
.890	12	3 1 2	119.97	
.863	1	2 0 5	126.39	
.846	1	4 0 1	131.21	
.843	14	3 0 4	131.93	
.826	2	3 1 3	137.53	
.812	8	4 0 2	143.29	
.809	8	1 0 6	144.59	
.7913	3	2 1 5	153.56	
.7779	5	3 2 1	163.92	

Cobalt germanium hafnium, $\text{Co}_{16}\text{Ge}_7\text{Hf}_6$

Structure

Cubic, $\text{Fm}3\text{m}$ (225), $Z = 4$, isostructural with $\text{Cu}_{16}\text{Mg}_6\text{Si}_7$, from powder data [Gladyshevs'kii et al., 1962].

Atom positions

The positions are those determined by Bergman and Waugh [1956] for $\text{Cu}_{16}\text{Mg}_6\text{Si}_7$.

32(f) 32 cobalt(1)
32(f) 32 cobalt(2)
24(e) 24 hafnium
4(b) 4 germanium(1)
24(d) 24 germanium(2)

Lattice constant

$a = 11.567 \text{ \AA}$
(published value, $a = 11.566$ [Gladyshevs'kii et al., 1962])

Volume \AA^3
 1547.6 \AA^3

Density
(calculated) 10.824 g/cm^3

Thermal parameters

Isotropic: cobalt, $B = 1.0$; germanium, $B = 1.0$;
hafnium, $B = 0.8$

Scattering factors

Co^0 , Ge^0 , Hf^0 [International Tables, 1962]

Scale factor (integrated intensities)
 $\gamma = 0.370 \times 10^{-3}$

References

Bergman, G. and Waugh, J. L. T. (1956). Acta Crystallogr. 9, 214.
Gladyshevs'kii, E. I., Markiv, V. Ya., and Kuz'ma, Yu.B. (1962). Dopov. Akad. Nauk. Ukr. RSR, No. 4, p. 481.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 204, 212.

Calculated Pattern (Peak heights)

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.540598\text{\AA}$
6.672	30	1 1 1	13.26
5.779	6	2 0 0	15.32
3.488	1	3 1 1	25.52
3.339	5	2 2 2	26.68
2.892	9	4 0 0	30.90
2.653	40	3 3 1	33.76
2.586	2	4 2 0	34.66
2.361	40	4 2 2	38.08
2.226	100	3 3 3+	40.50
2.045	55	4 4 0	44.26
1.955	8	5 3 1	46.40
1.928	30	6 0 0+	47.10
1.743	7	6 2 2	52.44
1.620	8	5 5 1	56.80
1.604	3	6 4 0	57.40
1.506	4	7 3 1+	61.54
1.446	5	8 0 0	64.38
1.413	8	7 3 3	66.06
1.403	1	6 4 4+	66.62
1.363	25	8 2 2+	68.82
1.336	11	7 5 1+	70.44
1.327	5	6 6 2	70.98
1.270	4	7 5 3+	74.70
1.262	11	8 4 2	75.24
1.181	1	8 4 4	81.46
1.163	18	9 3 3	83.00
1.157	2	10 0 0	83.50
1.134	1	8 6 2+	85.56
1.118	2	7 7 3+	87.08
1.113	7	6 6 6	87.58
1.079	1	9 5 3	91.14
1.074	1	10 4 0	91.66
1.043	3	11 1 1+	95.22
1.022	1	8 8 0	97.78
1.011	2	9 7 1	99.32
1.007	5	8 8 2	99.84
.992	1	10 6 0	101.90
.981	1	9 7 3	103.46
.978	5	10 6 2	103.98
.964	4	8 8 4+	106.10
.954	4	11 5 1	107.68
.938	2	10 6 4+	110.38
.914	5	12 4 0	114.78
.903	1	8 8 6+	117.04
.8924	2	10 8 2	119.34
.8845	11	11 5 5+	121.12
.8823	8	10 6 6	121.64
.8645	6	13 3 1+	126.00
.8622	7	12 6 0+	126.60
.8458	2	13 3 3	131.20

Cobalt germanium hafnium, Co₁₆Ge₇Hf₆ - (Continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
6.678	40	1 1 1	13.25	
5.783	8	2 0 0	15.31	
4.090	1	2 2 0	21.71	
3.488	2	3 1 1	25.52	
3.339	8	2 2 2	26.68	
2.892	15	4 0 0	30.90	
2.654	65	3 3 1	33.75	
2.586	2	4 2 0	34.65	
2.361	70	4 2 2	38.08	
2.226	80	5 1 1	40.49	
2.226	95	3 3 3	40.49	
2.045	100	4 4 0	44.26	
1.955	14	5 3 1	46.40	
1.928	40	6 0 0	47.10	
1.928	17	4 4 2	47.10	
1.744	14	6 2 2	52.43	
1.620	15	5 5 1	56.79	
1.604	6	6 4 0	57.40	
1.506	6	7 3 1	61.53	
1.506	2	5 5 3	61.53	
1.446	9	8 0 0	64.38	
1.413	16	7 3 3	66.06	
1.403	1	6 4 4	66.62	
1.363	20	6 6 0	68.81	
1.363	25	8 2 2	68.81	
1.336	13	7 5 1	70.44	
1.336	9	5 5 5	70.44	
1.327	9	6 6 2	70.98	
1.270	2	9 1 1	74.70	
1.270	7	7 5 3	74.70	
1.262	20	8 4 2	75.23	
1.233	1	6 6 4	77.32	
1.181	3	8 4 4	81.46	
1.163	35	9 3 3	83.00	
1.163	2	7 5 5	83.00	
1.157	2	10 0 0	83.51	
1.134	1	8 6 2	85.55	
1.134	1	10 2 0	85.55	
1.118	3	7 7 3	87.08	
1.118	1	9 5 1	87.08	
1.113	13	6 6 6	87.59	
1.079	2	9 5 3	91.15	
1.074	2	10 4 0	91.66	
1.056	1	10 4 2	93.69	
1.043	6	11 1 1	95.22	
1.043	1	7 7 5	95.22	
1.022	2	8 8 0	97.78	
1.011	4	9 7 1	99.32	
1.007	11	8 8 2	99.83	
.992	3	10 6 0	101.90	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
.981	3	9 7 3	103.47	
.978	11	10 6 2	103.99	
.964	5	8 8 4	106.10	
.964	4	12 0 0	106.10	
.954	8	11 5 1	107.69	
.938	1	12 2 2	110.38	
.938	3	10 6 4	110.38	
.929	1	11 5 3	112.01	
.914	11	12 4 0	114.78	
.906	1	9 9 1	116.47	
.903	1	8 8 6	117.04	
.8924	5	10 8 2	119.35	
.8846	11	11 5 5	121.11	
.8846	5	11 7 1	121.11	
.8846	11	9 9 3	121.11	
.8820	10	10 6 6	121.71	
.8646	10	13 3 1	125.99	
.8646	2	11 7 3	125.99	
.8646	3	9 7 7	125.99	
.8622	12	12 6 0	126.62	
.8622	3	10 8 4	126.62	
.8459	5	13 3 3	131.20	

Cobalt germanium niobium, $\text{Co}_{16}\text{Ge}_7\text{Nb}_6$

Structure

Cubic, $\text{Fm}\bar{3}\text{m}$ (225), $Z = 4$, isostructural with $\text{Cu}_{16}\text{Mg}_6\text{Si}_7$, from powder data [Spiegel et al., 1963]. Kuz'ma et al. [1964] determined positions for $\text{Co}_{16}\text{Nb}_6\text{Si}_7$, a similar isostructural compound.

Atom positions

From considerations of atomic size, the positions of $\text{Co}_{16}\text{Nb}_6\text{Si}_7$ were preferred.

- 32(f) 32 cobalt (1)
 32(f) 32 cobalt (2)
 4(b) 4 germanium (1)
 24(d) 24 germanium (2)
 24(e) 24 niobium

Lattice constant

$a = 11.477 \text{ \AA}$
 (published value, 11.478 \AA [Spiegel et al., 1963])

Volume

1511.8 \AA^3

Density

(calculated) 8.825 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Scattering factors

Co^0 , Ge^0 , Nb^0 [International Tables, 1962]

Scale factor (integrated intensities)

$\gamma = 0.425 \times 10^{-3}$

References

- International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.), pp. 204, 211.
 Kuz'ma, Yu. B., Gladyshevs'kii, E. I., and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.
 Spiegel, F. X., Bardos, D., and Beck, P. A. (1963). Trans. AIME 227, 575.

Calculated Pattern (Peak heights)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598 \text{ \AA}$
5.734	4	2 0 0	15.44	
3.458	2	3 1 1	25.74	
2.868	3	4 0 0	31.16	
2.633	19	3 3 1	34.02	
2.566	3	4 2 0	34.94	
2.342	30	4 2 2	38.40	
2.209	80	3 3 3+	40.82	
2.029	100	4 4 0	44.62	
1.940	17	5 3 1	46.80	
1.913	20	6 0 0+	47.50	
1.815	2	6 2 0	50.24	
1.750	3	5 3 3	52.22	
1.730	14	6 2 2	52.88	
1.607	4	5 5 1+	57.28	
1.494	5	7 3 1+	62.06	
1.434	6	8 0 0	64.96	
1.402	5	7 3 3	66.64	
1.352	15	8 2 2+	69.44	
1.325	7	5 5 5+	71.08	
1.317	3	6 6 2	71.62	
1.283	1	8 4 0	73.78	
1.260	7	7 5 3+	75.40	
1.252	7	8 4 2	75.92	
1.203	1	9 3 1	79.62	
1.171	7	8 4 4	82.24	
1.153	14	9 3 3	83.80	
1.148	2	8 6 0+	84.30	
1.125	1	10 2 0+	86.38	
1.109	3	7 7 3+	87.94	
1.104	7	6 6 6+	88.46	
1.066	1	10 4 0	92.58	
1.035	1	11 1 1	96.20	
1.014	3	8 8 0	98.82	
1.003	4	9 7 1+	100.38	
.9990	3	8 8 2	100.90	
.9841	1	8 6 6+	103.02	
.9700	7	10 6 2	105.14	
.9564	2	12 0 0+	107.30	
.9467	1	11 5 1+	108.92	
.9435	1	12 2 0	109.46	

Cobalt germanium niobium, Co₁₆Ge₇Nb₆ - (Continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
5.738	3	2 0 0	15.43	
3.460	2	3 1 1	25.72	
2.869	3	4 0 0	31.15	
2.633	17	3 3 1	34.02	
2.566	2	4 2 0	34.93	
2.343	30	4 2 2	38.39	
2.209	35	5 1 1	40.82	
2.209	40	3 3 3	40.82	
2.029	100	4 4 0	44.63	
1.940	17	5 3 1	46.79	
1.913	17	6 0 0	47.49	
1.913	4	4 4 2	47.49	
1.815	2	6 2 0	50.24	
1.750	3	5 3 3	52.22	
1.730	14	6 2 2	52.87	
1.607	1	7 1 1	57.28	
1.607	3	5 5 1	57.28	
1.494	4	7 3 1	62.07	
1.494	1	5 5 3	62.07	
1.435	7	8 0 0	64.95	
1.402	6	7 3 3	66.65	
1.353	9	8 2 2	69.43	
1.353	8	6 6 0	69.43	
1.325	4	7 5 1	71.08	
1.325	4	5 5 5	71.08	
1.317	3	6 6 2	71.62	
1.283	1	8 4 0	73.78	
1.260	1	9 1 1	75.39	
1.260	7	7 5 3	75.39	
1.252	7	8 4 2	75.92	
1.203	1	9 3 1	79.62	
1.171	8	8 4 4	82.24	
1.153	15	9 3 3	83.80	
1.153	1	7 7 1	83.80	
1.148	1	8 6 0	84.31	
1.125	1	10 2 0	86.39	
1.110	1	9 5 1	87.94	
1.110	2	7 7 3	87.94	
1.104	1	10 2 2	88.45	
1.104	6	6 6 6	88.45	
1.066	1	10 4 0	92.58	
1.035	2	11 1 1	96.21	
1.014	4	8 8 0	98.81	
1.003	3	9 7 1	100.38	
1.003	1	11 3 1	100.38	
.9989	4	8 8 2	100.91	
.9700	9	10 6 2	105.15	
.9564	1	8 8 4	107.30	
.9564	1	12 0 0	107.30	
.9466	1	11 5 1	108.93	
.9434	1	12 2 0	109.47	

Cobalt germanium tantalum, $\text{Co}_{16}\text{Ge}_7\text{Ta}_6$

Structure

Cubic, $\text{Fm}\bar{3}\text{m}$ (225), $Z = 4$, isostructural with $\text{Cu}_{16}\text{Mg}_6\text{Si}_7$, from powder data [Gladyshevs'kii et al., 1962]. Kuz'ma et al. [1964] determined positions for $\text{Co}_{16}\text{Nb}_6\text{Si}_7$, a similar isostructural compound.

Atom positions

From considerations of atomic size, the positions of $\text{Co}_{16}\text{Nb}_6\text{Si}_7$ were preferred.

32(f)	32 cobalt(1)
32(f)	32 cobalt(2)
4(b)	4 germanium(1)
24(d)	24 germanium(2)
24(e)	24 tantalum

Lattice constant

$a = 11.421 \text{ \AA}$
(published value, 11.420 \AA [Gladyshevs'kii et al., 1962]).

Volume

1489.8 \AA^3

Density

(calculated) 11.310 g/cm^3

Thermal parameters

Isotropic: cobalt $B = 1.0$; germanium $B = 1.0$;
tantalum $B = 0.8$.

Scattering factors

Co^0 , Ge^0 , Ta^0 [International Tables, 1962]

Scale factor (integrated intensities)

$\gamma = 0.463 \times 10^{-3}$

References

Gladyshevs'kii, E. I., Markiv, V. Ya., and Kuz'ma, Yu. B. (1962). Dopov. Akad. Nauk. Ukr. RSR, No. 4, p. 481.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 204, 212.

Kuz'ma, Yu. B., Gladyshevs'kii, E. I. and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.

Calculated Pattern (Peak heights)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
6.593	17	1 1 1	13.42	
5.705	4	2 0 0	15.52	
4.037	3	2 2 0	22.00	
3.443	2	3 1 1	25.86	
3.295	11	2 2 2	27.04	
2.855	14	4 0 0	31.30	
2.620	35	3 3 1	34.20	
2.553	4	4 2 0	35.12	
2.331	40	4 2 2	38.60	
2.198	100	3 3 3+	41.04	
2.019	75	4 4 0	44.86	
1.930	5	5 3 1	47.04	
1.904	25	6 0 0+	47.74	
1.722	3	6 2 2	53.16	
1.599	10	5 5 1	57.58	
1.584	3	6 4 0	58.20	
1.487	9	7 3 1+	62.40	
1.428	5	8 0 0	65.30	
1.395	11	7 3 3	67.02	
1.385	2	6 4 4+	67.58	
1.346	25	8 2 2+	69.82	
1.319	10	5 5 5+	71.48	
1.310	2	6 6 2	72.02	
1.254	5	7 5 3	75.82	
1.246	10	8 4 2	76.36	
1.166	3	8 4 4	82.72	
1.148	15	9 3 3+	84.30	
1.142	2	10 0 0	84.82	
1.120	3	8 6 2+	86.92	
1.104	6	7 7 3+	88.48	
1.099	5	6 6 6	89.00	
1.060	3	10 4 0	93.18	
1.030	2	11 1 1	96.84	
1.009	1	8 8 0	99.48	
.998	3	9 7 1+	101.06	
.994	6	8 8 2	101.60	
.979	2	10 6 0	103.72	
.969	1	9 7 3	105.34	
.965	6	10 6 2	105.88	
.952	3	8 8 4+	108.06	
.942	4	11 5 1+	109.72	

Cobalt germanium tantalum, Co₁₆Ge₇Ta₆ - (Continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
6.594	19	1 1 1	13.42	
5.711	5	2 0 0	15.50	
4.038	4	2 2 0	21.99	
3.444	3	3 1 1	25.85	
3.297	13	2 2 2	27.02	
2.855	17	4 0 0	31.30	
2.620	45	3 3 1	34.19	
2.554	5	4 2 0	35.11	
2.331	50	4 2 2	38.59	
2.198	65	5 1 1	41.03	
2.198	70	3 3 3	41.03	
2.019	100	4 4 0	44.86	
1.931	7	5 3 1	47.03	
1.904	30	6 0 0	47.74	
1.904	6	4 4 2	47.74	
1.722	5	6 2 2	53.15	
1.599	15	5 5 1	57.59	
1.584	4	6 4 0	58.20	
1.487	10	7 3 1	62.40	
1.487	3	5 5 3	62.40	
1.428	7	8 0 0	65.31	
1.395	16	7 3 3	67.02	
1.385	1	8 2 0	67.58	
1.385	2	6 4 4	67.58	
1.346	13	6 6 0	69.82	
1.346	20	8 2 2	69.82	
1.319	6	7 5 1	71.48	
1.319	9	5 5 5	71.48	
1.310	3	6 6 2	72.03	
1.277	1	8 4 0	74.21	
1.254	7	7 5 3	75.83	
1.246	16	8 4 2	76.36	
1.166	4	8 4 4	82.73	
1.148	20	9 3 3	84.30	
1.148	2	7 7 1	84.30	
1.148	1	7 5 5	84.30	
1.142	2	10 0 0	84.82	
1.120	3	8 6 2	86.91	
1.120	2	10 2 0	86.91	
1.104	6	7 7 3	88.48	
1.104	4	9 5 1	88.48	
1.099	8	6 6 6	89.00	
1.060	4	10 4 0	93.17	
1.030	4	11 1 1	96.84	
1.009	2	8 8 0	99.47	
.998	1	11 3 1	101.06	
.998	3	9 7 1	101.06	
.994	1	10 4 4	101.59	
.994	9	8 8 2	101.59	
.979	3	10 6 0	103.73	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
.969	2	9 7 3	105.34	
.965	10	10 6 2	105.88	
.952	2	12 0 0	108.07	
.952	3	8 8 4	108.07	
.942	6	11 5 1	109.72	
.942	1	7 7 7	109.72	

Cobalt hafnium tin, Co₂HfSn

Structure

Cubic, Fm3m (225), Z = 4, a Heusler alloy iso-structural with AlCu₂Mn, from powder data (x-ray and neutron) [Ziebeck and Webster, 1974].

Atom positions

8(c) 8 cobalt
4(b) 4 hafnium
4(a) 4 tin

Lattice constant

a = 6.218 Å [Table 1, Ziebeck and Webster, 1974].

Volume

240.41 Å³

Density

(calculated) 11.466 g/cm³
(measured) 11.400 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co⁰ Sn⁰ [Cromer and Mann, 1968]

Hf⁰ [International Tables, 1974]

All factors were corrected for anomalous dispersion [Cromer and Liberman, 1970].

Scale factor (integrated intensities)

$\gamma = 1.253 \times 10^{-3}$

References

Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.

Cromer, D.T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.

International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.

Ziebeck, K.R.A. and Webster, P.J. (1974). J. Phys. Chem. Solids 35, 1.

Calculated Pattern (Peak heights)

d (Å)	I	hkl	2θ (°)
$\lambda = 1.540598 \text{ Å}$			
3.590	5	1 1 1	24.78
3.108	25	2 0 0	28.70
2.199	100	2 2 0	41.02
1.875	1	3 1 1	48.52
1.795	5	2 2 2	50.82
1.554	15	4 0 0	59.42
1.390	5	4 2 0	67.28
1.269	20	4 2 2	74.74
1.099	5	4 4 0	88.98
1.036	5	4 4 2	96.02
.9832	10	6 2 0	103.16
.9374	1	6 2 2	110.52
.8975	1	4 4 4	118.24
.8623	1	6 4 0	126.58
.8309	10	6 4 2	135.96

Calculated Pattern (Integrated)

d (Å)	I	hkl	2θ (°)
$\lambda = 1.540598 \text{ Å}$			
3.590	5	1 1 1	24.78
3.109	25	2 0 0	28.69
2.198	100	2 2 0	41.02
1.875	1	3 1 1	48.52
1.795	5	2 2 2	50.83
1.554	15	4 0 0	59.41
1.390	10	4 2 0	67.29
1.269	25	4 2 2	74.73
1.099	5	4 4 0	88.98
1.036	5	4 4 2	96.03
1.036	1	6 0 0	96.03
.9832	10	6 2 0	103.16
.9374	5	6 2 2	110.52
.8975	5	4 4 4	118.25
.8623	5	6 4 0	126.59
.8309	25	6 4 2	135.96

Cobalt holmium, Co₂Ho

Structure

Cubic, Fd3m (227), Z = 8, isostructural with Cu₂Mg, from powder data [Harris et al., 1965].

Atom positions [ibid.]

8(a) 8 holmium

16(d) 16 cobalt

Lattice constant [ibid.]

a = 7.1734 Å

(published value, 7.1585 kX)

Volume

369.1 Å³

Density

(calculated) 10.177 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co⁰, Ho⁰ [Cromer and Mann, 1968]

Scale factor (integrated intensities)

$\gamma = 1.07 \times 10^{-3}$

References

Cromer, D. T. and Mann, J. B. (1968). Acta Cryst-allogr. A24, 321.

Harris, I. R., Mansey, R. C., and Raynor, G. V. (1965). J. Less-Common Metals 9, 270.

Calculated Pattern (Integrated)

d(Å)	I	hkl	2θ(°)
λ = 1.540598Å			
4.142	17	1 1 1	21.44
2.536	70	2 2 0	35.36
2.163	100	3 1 1	41.73
2.071	14	2 2 2	43.68
1.7934	1	4 0 0	50.88
1.6457	4	3 3 1	55.82
1.4643	20	4 2 2	63.48
1.3805	20	5 1 1	67.83
1.3805	7	3 3 3	67.83
1.2681	18	4 4 0	74.81
1.2125	3	5 3 1	78.88
1.1342	8	6 2 0	85.55
1.0939	8	5 3 3	89.52
1.0814	3	6 2 2	90.84
1.0045	1	7 1 1	100.15
1.0045	1	5 5 1	100.15
.9586	11	6 4 2	106.95
.9339	12	7 3 1	111.14
.9339	6	5 5 3	111.14
.8967	4	8 0 0	118.42
.8764	1	7 3 3	123.04
.8454	3	6 6 0	131.34
.8454	6	8 2 2	131.34
.8283	13	7 5 1	136.86
.8283	2	5 5 5	136.86
.8228	3	6 6 2	138.83
.8020	1	8 4 0	147.67
.7874	4	7 5 3	156.09
.7874	2	9 1 1	156.09

Calculated Pattern (Peak heights)

d(Å)	I	hkl	2θ(°)
λ = 1.540598Å			
4.141	20	1 1 1	21.44
2.536	70	2 2 0	35.36
2.162	100	3 1 1	41.74
2.071	14	2 2 2	43.68
1.7932	1	4 0 0	50.88
1.6456	4	3 3 1	55.82
1.4643	20	4 2 2	63.48
1.3804	25	5 1 1+	67.84
1.2680	16	4 4 0	74.82
1.2126	3	5 3 1	78.88
1.1342	7	6 2 0	85.56
1.0940	7	5 3 3	89.52
1.0815	3	6 2 2	90.84
1.0045	1	7 1 1+	100.14
.9586	9	6 4 2	106.94
.9339	13	7 3 1+	111.14
.8967	3	8 0 0	118.42
.8454	5	8 2 2+	131.34
.8283	8	7 5 1+	136.86
.8229	1	6 6 2	138.82
.7874	2	7 5 3+	156.08

Cobalt iron sulfide, Co_8FeS_8

Structure

Cubic, $\text{Fm}\bar{3}\text{m}$ (225), $Z = 4$, π phase, isostructural with Co_9S_8 , from powder data (neutron and x-ray) [Knop, 1962].

Atom positions [Pearson, 1967]

4(b) 3.6 cobalt 32(f) 3.6 iron
4(b) 0.4 iron 24(e) 8.0 sulfur
32(f) 28.4 cobalt 24(e) 24.0 sulfur

Lattice constant

$a = 9.944(2) \text{ \AA}$
(published value, $a = 9.943(2) \text{ \AA}$, [Knop, 1962])

Volume

983.3 \AA^3

Density

(calculated) 5.295 g/cm^3

Thermal parameters

Isotropic: cobalt, $B = 0.5$; iron, $B = 0.5$;
sulfur, $B = 0.7$

Scattering factors

Co^0 , Fe^0 , S^0 [International Tables, 1962]

Scale factors (integrated intensities)

$\gamma = 0.319 \times 10^{-3}$

References

- International Tables for X-ray Crystallography III
(1962). (The Kynoch Press, Birmingham, England).
pp. 202, 204.
Knop, D. (1962). Chem. Ind. London, April 21, p. 739.
Pearson, W.B. (1967). Handbook of Lattice Spacings and Structures of Metals and Alloys, v.2, (Pergamon, Press, N.Y.) pp. 197, 788.

Calculated Pattern (Peak heights)

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.540598\text{\AA}$
5.734	35	1 1 1	15.44
4.968	6	2 0 0	17.84
3.515	6	2 2 0	25.32
2.998	100	3 1 1	29.78
2.870	25	2 2 2	31.14
2.486	8	4 0 0	36.10
2.281	14	3 3 1	39.48
2.223	3	4 2 0	40.54
2.030	2	4 2 2	44.60
1.913	35	5 1 1+	47.48
1.758	95	4 4 0	51.98
1.681	5	5 3 1	54.56
1.657	1	4 4 2+	55.40
1.572	1	6 2 0	58.68
1.516	9	5 3 3	61.06
1.499	5	6 2 2	61.84
1.435	2	4 4 4	64.92
1.392	3	7 1 1+	67.18
1.329	1	6 4 2	70.86
1.2947	13	7 3 1+	73.02
1.2429	11	8 0 0	76.60
1.2149	2	7 3 3	78.70
1.1483	7	7 5 1+	84.26
1.1406	2	6 6 2	84.96
1.1117	1	8 4 0	87.72
1.0915	2	7 5 3	89.78
1.0425	5	9 3 1	95.28
1.0148	20	8 4 4	98.76
.9994	2	7 7 1+	100.84
.9614	6	9 5 1+	106.50
.9569	2	10 2 2+	107.22
.8966	2	11 1 1+	118.44
.8789	8	8 8 0	122.42
.8688	2	11 3 1+	124.90
.8435	3	9 7 3+	131.92
.8404	2	10 6 2	132.86
.8286	1	8 8 4+	136.74
.8202	1	11 5 1+	139.84
.7987	5	9 7 5+	149.34
.7861	17	12 4 0	156.96

Cobalt iron sulfide, Co_8FeS_8 - (continued)

Calculated Pattern (Integrated)					
$d(\text{\AA})$	I	hkl			$2\theta(^{\circ})$ $\lambda = 1.540598\text{\AA}$
5.741	25	1	1	1	15.42
4.972	5	2	0	0	17.83
3.516	5	2	2	0	25.31
2.998	90	3	1	1	29.77
2.871	20	2	2	2	31.13
2.486	7	4	0	0	36.10
2.281	14	3	3	1	39.47
2.224	3	4	2	0	40.54
2.030	2	4	2	2	44.60
1.914	30	5	1	1	47.47
1.914	6	3	3	3	47.47
1.758	100	4	4	0	51.98
1.681	5	5	3	1	54.55
1.657	1	4	4	2	55.39
1.572	1	6	2	0	58.67
1.516	10	5	3	3	61.06
1.499	6	6	2	2	61.84
1.435	2	4	4	4	64.92
1.392	2	7	1	1	67.17
1.329	1	6	4	2	70.86
1.2946	8	7	3	1	73.03
1.2946	6	5	5	3	73.03
1.2430	13	8	0	0	76.59
1.2149	2	7	3	3	78.70
1.1482	7	7	5	1	84.27
1.1482	2	5	5	5	84.27
1.1407	2	6	6	2	84.96
1.1118	2	8	4	0	87.71
1.0915	2	7	5	3	89.78
1.0424	6	9	3	1	95.29
1.0149	30	8	4	4	98.75
.9994	1	7	7	1	100.84
.9613	1	7	7	3	106.51
.9613	6	9	5	1	106.51
.9569	2	10	2	2	107.23
.8966	2	11	1	1	118.43
.8966	2	7	7	5	118.43
.8789	13	8	8	0	122.42
.8688	2	11	3	1	124.90
.8688	1	9	7	1	124.90
.8434	4	9	7	3	131.93
.8434	1	11	3	3	131.93
.8404	3	10	6	2	132.86
.8287	1	8	8	4	136.73
.8202	2	11	5	1	139.83
.8202	1	7	7	7	139.83
.7987	8	9	7	5	149.34
.7987	5	11	5	3	149.34
.7861	50	12	4	0	156.96

Structure

Tetragonal, $P4_2/mnm(136)$, $Z = 1$, σ -phase, iso-structural with σ -(Cr,Fe), from powder data [Stüwe, 1959]. Much work has been done on the σ -phase structure which has multiple atoms in 5 sites, called A through E [Bergman and Shoemaker, 1954]. The ordering arrangement of the atoms is dependent on a complex combination of electronic and size factors [Spoonner, 1968].

Atom positions

The positions used were those for σ -(Cr,Fe) [Spoonner and Wilson, 1964]. Site occupancy shared by multiple atoms was assumed to be random and in the following proportions:

Site A: 2(a) 0.49 cobalt and 1.51 iron

Site B: 4(f) 4.0 vanadium

Site C: 8(i) 7.0 vanadium, 0.24 cobalt, and 0.76 iron

Site D: 8(i) 1.95 cobalt and 6.05 iron

Site E: 8(j) 1.66 cobalt, 5.16 iron, and 1.18 vanadium

Lattice constants [Stüwe, 1959]

$a = 8.884 \text{ \AA}$

$c = 4.600$

Volume 363.1 \AA^3

Density

(calculated) 7.45 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Scattering factors

Co^0 , Fe^0 , V^0 [Cromer and Mann, 1968].

Scale factor (integrated intensities)

$\gamma = 0.136 \times 10^{-3}$

References

Bergman, G. and Shoemaker, D.P. (1954). Acta Crystallogr. 7, 857.

Cromer, D.T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.

Spoonner, F. J. (1968). Acta Crystallogr. A24, 605.

Spoonner, F. J. and Wilson, C. G. (1964). Acta Crystallogr. 17, 1533.

Stüwe, H. P. (1959). Trans. AIME 215, 408.

Calculated Pattern (Peak heights)

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.540598\text{\AA}$
4.085	8	1 0 1	21.74
3.711	2	1 1 1	23.96
2.398	4	3 1 1	37.48
2.300	20	0 0 2	39.14
2.154	100	4 1 0	41.90
2.094	40	3 3 0	43.16
2.042	35	2 0 2	44.32
1.990	70	2 1 2	45.54
1.951	95	4 1 1	46.50
1.906	50	3 3 1	47.68
1.855	13	2 2 2	49.06
1.780	15	3 1 2	51.30
1.681	4	3 2 2	54.54
1.658	4	4 3 1	55.38
1.630	4	5 1 1	56.42
1.598	1	4 0 2	57.64
1.553	1	5 2 1	59.48
1.406	2	4 3 2	66.44
1.389	2	5 1 2	67.38
1.341	4	5 2 2	70.14
1.2703	12	5 3 2	74.66
1.2565	5	5 5 0	75.62
1.2492	14	4 1 3	76.14
1.2459	11	6 0 2	76.38
1.2371	8	3 3 3	77.02
1.2331	7	6 1 2	77.32
1.2203	11	7 2 0	78.28
1.2120	6	5 5 1	78.92
1.1989	4	6 2 2	79.96
1.1880	4	5 4 2	80.84
1.1796	7	7 2 1	81.54
1.1609	1	4 3 3	83.14
1.1501	7	0 0 4	84.10
1.0774	7	8 2 0	91.28
1.0490	3	8 2 1	94.50
1.0470	4	6 6 0	94.74
1.0210	2	6 6 1	97.96
1.0145	9	4 1 4	98.80
1.0081	4	3 3 4	99.66
1.0000	3	8 0 2	100.76
.9939	7	7 4 2	101.62
.9757	2	8 2 2	104.28
.9719	3	5 5 3	104.86
.9548	3	7 2 3	107.56
.9431	1	7 6 1+	109.52
.8887	2	7 6 2+	120.16
.8816	2	8 2 3	121.80
.8674	2	9 3 2	125.26
.8647	2	6 6 3	125.96
.8483	3	5 5 4	130.48

Cobalt iron vanadium, $\text{Co}_{4.35}\text{Fe}_{13.47}\text{V}_{12.18}$ - (continued)

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
.8461	5	4 1 5	131.12	
.8423	2	3 3 5	132.28	
.8398	3	9 4 2	133.04	
.8369	7	7 2 4	133.96	
.8337	1	8 4 3	135.02	
.8288	2	8 6 2+	136.70	
.8252	2	10 1 2	137.98	
.8214	2	9 6 0	139.38	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
4.085	7	1 0 1	21.74	
3.711	2	1 1 1	23.96	
2.398	4	3 1 1	37.48	
2.300	20	0 0 2	39.13	
2.160	2	1 1 2	41.79	
2.155	100	4 1 0	41.89	
2.094	45	3 3 0	43.17	
2.042	35	2 0 2	44.31	
1.991	75	2 1 2	45.53	
1.987	1	4 2 0	45.63	
1.951	100	4 1 1	46.50	
1.906	50	3 3 1	47.68	
1.856	13	2 2 2	49.05	
1.780	15	3 1 2	51.29	
1.681	4	3 2 2	54.53	
1.658	4	4 3 1	55.38	
1.629	4	5 1 1	56.43	
1.598	1	4 0 2	57.65	
1.553	1	5 2 1	59.47	
1.406	2	4 3 2	66.43	
1.389	2	5 1 2	67.37	
1.344	1	6 2 1	69.97	
1.341	4	5 2 2	70.14	
1.2702	14	5 3 2	74.66	
1.2565	5	5 5 0	75.62	
1.2493	16	4 1 3	76.13	
1.2450	8	6 0 2	76.44	
1.2371	9	3 3 3	77.02	
1.2330	6	6 1 2	77.33	
1.2235	1	7 0 1	78.04	
1.2204	12	7 2 0	78.28	
1.2121	7	5 5 1	78.92	
1.1988	4	6 2 2	79.96	
1.1901	1	6 4 1	80.67	
1.1881	4	5 4 2	80.84	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
1.1796	9	7 2 1	81.54	
1.1609	1	4 3 3	83.14	
1.1511	1	5 1 3	84.01	
1.1500	7	0 0 4	84.11	
1.1477	1	6 3 2	84.31	
1.0780	1	7 2 2	91.21	
1.0774	8	8 2 0	91.28	
1.0490	4	8 2 1	94.50	
1.0470	3	6 6 0	94.73	
1.0209	3	6 6 1	97.96	
1.0146	11	4 1 4	98.80	
1.0080	5	3 3 4	99.67	
1.0001	4	8 0 2	100.75	
.9938	8	7 4 2	101.63	
.9757	2	8 2 2	104.28	
.9719	3	5 5 3	104.86	
.9709	1	8 4 1	105.00	
.9549	4	7 2 3	107.55	
.8888	1	9 2 2	120.15	
.8888	1	7 6 2	120.15	
.8815	3	8 2 3	121.81	
.8674	3	9 3 2	125.27	
.8647	2	6 6 3	125.96	
.8483	4	5 5 4	130.47	
.8461	7	4 1 5	131.12	
.8423	4	3 3 5	132.28	
.8398	5	9 4 2	133.05	
.8369	11	7 2 4	133.96	
.8368	1	10 3 1	134.01	
.8337	1	8 4 3	135.03	
.8288	4	8 6 2	136.70	
.8288	1	10 0 2	136.70	
.8252	4	10 1 2	137.97	
.8214	4	9 6 0	139.38	

Cobalt manganese silicide, Co₂MnSi

Structure

Cubic, Fm3m (225), Z = 4, a Heusler alloy, isostructural with AlCu₂Mn, from powder data [Gladyshevs'kii et al., 1962].

Atom positions

8(c) 8 cobalt
4(b) 4 manganese
4(a) 4 silicon

Lattice constant

a = 5.670 Å [Gladyshevs'kii et al., 1962]

Volume

182.3 Å³

Density

(calculated) 7.320 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co⁰, Mn⁰, Si⁰ [Cromer and Mann, 1968]

Scale factor (integrated intensities)

γ = 0.599 × 10⁻³

References

Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.
Gladyshevs'kii, E.I., Kripyakevich, P.I., Teslyuk, M.Yu., Zarechnyuk, O. S. and Kuz'ma, Yu.B. (1962). Sov. Phys. Crystallogr. 6, 207.

Calculated Pattern (Peak Heights)

d(Å)	I	hkl	2θ(°)
λ = 1.540598Å			
3.274	5	1 1 1	27.22
2.834	5	2 0 0	31.54
2.004	100	2 2 0	45.20
1.710	1	3 1 1	53.56
1.636	1	2 2 2	56.16
1.417	10	4 0 0	65.84
1.268	1	4 2 0	74.82
1.157	20	4 2 2	83.44
1.002	5	4 4 0	100.44
.8965	10	6 2 0	118.46
.8184	1	4 4 4	140.52

Calculated Pattern (Integrated)

d(Å)	I	hkl	2θ(°)
λ = 1.540598Å			
3.274	5	1 1 1	27.22
2.835	5	2 0 0	31.53
2.005	100	2 2 0	45.20
1.710	1	3 1 1	53.56
1.637	1	2 2 2	56.15
1.418	15	4 0 0	65.83
1.268	1	4 2 0	74.83
1.157	20	4 2 2	83.45
1.002	5	4 4 0	100.44
.8965	10	6 2 0	118.46
.8184	5	4 4 4	140.52

Cobalt molybdenum, Co₃Mo

Structure

Hexagonal, P6₃/mmc (194), Z = 2, isostructural with Ni₃Sn. The structure was determined by Alte da Veiga [1965].

Atom positions

6(h) 6 cobalt
2(c) 2 molybdenum

Lattice constants

a = 5.125 Å
c = 4.113
(published values: a = 5.1245 [±.0015] and c = 4.1125 [±.0020]) [Alte da Veiga, 1965].

c/a = 0.8025

Volume

93.56 Å³

Density

(calculated) 9.682 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co²⁺, Mo⁺ [Forsyth and Wells, 1959]; corrected for dispersion using Δf' values from Dauben and Templeton [1955].

Scale factors (integrated intensities)

γ = 0.468 × 10⁻³

I/I_c (calculated) = 7.6

References

Alte da Veiga, L.H. (1965). Acta Crystallogr. **18**, 857.
Dauben, C. H., and Templeton, D. H. (1955). Acta Crystallogr. **8**, 841.
Forsyth, J.B. and Wells, M. (1959). Acta Crystallogr. **12**, 412.

Calculated Pattern (Peak heights)

d(Å)	I	hkl	2θ(°)
λ = 1.540598 Å			
4.436	3	1 0 0	20.00
3.016	12	1 0 1	29.60
2.562	4	1 1 0	35.00
2.219	27	2 0 0	40.62
2.056	27	0 0 2	44.00
1.953	100	2 0 1	46.46
1.677	1	2 1 0	54.68
1.604	2	1 1 2	57.40
1.553	2	2 1 1	59.46
1.508	11	2 0 2	61.42
1.310	1	1 0 3	72.04
1.300	1	2 1 2	72.68
1.281	11	2 2 0	73.92
1.179	1	3 1 1	81.56
1.166	11	2 0 3	82.66

d(Å)	I	hkl	2θ(°)
λ = 1.540598 Å			
1.109	1	4 0 0	87.94
1.087	11	2 2 2	90.20
1.071	7	4 0 1	91.96
1.028	1	0 0 4	97.04
.988	1	3 2 1	102.40
.976	2	4 0 2	104.16
.933	2	2 0 4	111.30
.876	1	4 1 2	123.06
.863	4	4 0 3	126.52
.8388	1	4 2 0	133.38
.8218	7	4 2 1	139.20
.8174	1	3 2 3	140.90
.8019	5	2 2 4	147.70

Calculated Pattern (Integrated)

d(Å)	I	hkl	2θ(°)
λ = 1.540598 Å			
4.438	3	1 0 0	19.99
3.017	11	1 0 1	29.59
2.563	4	1 1 0	34.99
2.219	26	2 0 0	40.62
2.056	27	0 0 2	44.00
1.953	100	2 0 1	46.46
1.678	1	2 1 0	54.67
1.604	2	1 1 2	57.41
1.553	2	2 1 1	59.46
1.508	12	2 0 2	61.42
1.310	1	1 0 3	72.04
1.300	1	2 1 2	72.68
1.281	12	2 2 0	73.91
1.201	1	3 0 2	79.79
1.179	1	3 1 1	81.56
1.166	12	2 0 3	82.66
1.110	2	4 0 0	87.93
1.087	12	2 2 2	90.20
1.071	9	4 0 1	91.95
1.028	2	0 0 4	97.03
.988	1	3 2 1	102.40
.977	2	4 0 2	104.15
.933	2	2 0 4	111.31
.916	1	3 1 3	114.49
.876	1	4 1 2	123.07
.863	6	4 0 3	126.53
.8388	2	4 2 0	133.38
.8219	15	4 2 1	139.19
.8174	1	3 2 3	140.89
.8019	12	2 2 4	147.71

Cobalt phosphide, CoP

Structure

Orthorhombic, Pnma (62), $Z = 4$, isostructural with MnP. The structure was refined by Rundqvist [1962].

Atom positions

All atoms were located in positions 4(c).

Lattice constants

$a = 5.077 \text{ \AA}$

$b = 3.281$

$c = 5.587$

[Rundqvist, 1962].

CD cell: $a = 5.077$, $b = 5.587$, $c = 3.281$, space group Pnam, $a/b = 0.9087$, $c/b = 0.5873$.

Volume

93.07 \AA^3

Density

(calculated) 6.417 g/cm^3

Thermal parameters

Isotropic: overall $B = 0.29$

Scattering factors

Co^0 , P^0 [International Tables, 1962]. The cobalt factors were corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)

$\gamma = 0.158 \times 10^{-3}$

I/I_c (calculated) = 2.28

References

Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. **8**, 841.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 210.

Rundqvist, S. (1962). Acta Chem. Scand. **16**, 287.

Calculated Pattern (Peak heights)

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$
$\lambda = 1.540598\text{\AA}$			
3.757	7	1 0 1	23.66
2.829	68	0 1 1	31.60
2.793	20	0 0 2	32.02
2.538	18	2 0 0	35.34
2.472	41	1 1 1	36.32
2.447	20	1 0 2	36.70
2.311	2	2 0 1	38.94
2.008	7	2 1 0	45.12
1.962	51	1 1 2	46.24
1.889	100	2 1 1	48.12
1.879	46	2 0 2	48.40
1.748	19	1 0 3	52.28
1.640	26	0 2 0	56.02
1.631	4	2 1 2	56.38
1.620	38	0 1 3+	56.80

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$
$\lambda = 1.540598\text{\AA}$			
1.502	3	2 0 3	61.72
1.452	1	3 1 1	64.06
1.415	3	0 2 2	65.98
1.378	3	2 2 0	67.98
1.363	5	1 2 2	68.84
1.347	2	1 0 4	69.78
1.338	1	2 2 1	70.32
1.269	4	4 0 0	74.74
1.253	5	3 0 3	75.90
1.246	9	1 1 4	76.38
1.236	14	2 2 2	77.12
1.224	2	2 0 4	78.02
1.196	8	1 2 3	80.16
1.184	2	4 1 0	81.20
1.158	9	4 1 1	83.40
1.155	8	4 0 2	83.64
1.153	9	3 2 1	83.88
1.108	2	2 2 3	88.12
1.091	6	1 0 5	89.80
1.073	2	0 3 1	91.72
1.050	2	1 3 1	94.38
1.049	2	4 0 3	94.52
1.041	2	1 2 4	95.46
1.036	2	1 1 5	96.12
1.023	15	3 1 4	97.64
1.004	4	4 2 0	100.22
.999	6	1 3 2+	100.96
.996	6	3 2 3	101.38
.989	9	2 3 1	102.38
.981	2	2 2 4	103.50
.945	4	4 2 2	109.24
.943	5	0 3 3	109.54
.932	1	3 0 5	111.40
.916	7	5 1 2	114.42
.909	8	1 2 5	115.94
.892	2	5 0 3	119.54
.884	3	4 2 3	121.32
.882	5	1 1 6	121.66
.874	2	2 0 6	123.56
.8490	3	1 3 4	130.28
.8462	3	6 0 0	131.10
.8447	1	2 1 6	131.54
.8285	1	4 3 0	136.78
.8202	4	0 4 0	139.82
.8195	5	4 3 1+	140.08
.8107	4	6 1 1+	143.68
.8098	2	6 0 2+	144.04
.7967	1	5 1 4	150.40
.7943	1	4 3 2	151.74
.7917	4	3 1 6	153.28

Cobalt phosphide, CoP - (Continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
3.757	6	1 0 1	23.66	
2.829	62	0 1 1	31.60	
2.794	17	0 0 2	32.01	
2.539	17	2 0 0	35.33	
2.471	38	1 1 1	36.32	
2.447	18	1 0 2	36.69	
2.311	2	2 0 1	38.94	
2.008	7	2 1 0	45.12	
1.962	52	1 1 2	46.24	
1.889	100	2 1 1	48.12	
1.879	38	2 0 2	48.41	
1.748	20	1 0 3	52.28	
1.640	28	0 2 0	56.01	
1.630	2	2 1 2	56.39	
1.620	12	3 0 1	56.80	
1.620	28	0 1 3	56.80	
1.502	2	2 0 3	61.73	
1.452	2	3 1 1	64.06	
1.415	3	0 2 2	65.99	
1.378	4	2 2 0	67.98	
1.363	5	1 2 2	68.84	
1.347	3	1 0 4	69.78	
1.338	1	2 2 1	70.31	
1.269	5	4 0 0	74.73	
1.252	5	3 0 3	75.91	
1.246	9	1 1 4	76.38	
1.238	1	4 0 1	76.98	
1.236	16	2 2 2	77.13	
1.224	2	2 0 4	78.02	
1.196	9	1 2 3	80.16	
1.184	2	4 1 0	81.19	
1.158	10	4 1 1	83.39	
1.156	4	4 0 2	83.61	
1.153	8	3 2 1	83.88	
1.108	2	2 2 3	88.12	
1.091	7	1 0 5	89.80	
1.090	1	4 1 2	89.94	
1.073	2	0 3 1	91.73	
1.058	1	0 1 5	93.48	
1.050	2	1 3 1	94.37	
1.049	2	4 0 3	94.52	
1.041	2	1 2 4	95.47	
1.036	2	1 1 5	96.13	
1.023	18	3 1 4	97.64	
1.004	1	2 3 0	100.16	
1.004	5	4 2 0	100.23	
.999	3	4 1 3	100.90	
.999	5	1 3 2	100.97	
.995	5	3 2 3	101.39	
.989	11	2 3 1	102.38	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
.988	1	4 2 1	102.45	
.981	2	2 2 4	103.50	
.945	4	4 2 2	109.25	
.943	6	0 3 3	109.53	
.932	1	3 0 5	111.40	
.916	10	5 1 2	114.41	
.909	11	1 2 5	115.94	
.891	3	5 0 3	119.55	
.884	3	4 2 3	121.32	
.882	7	1 1 6	121.66	
.874	3	2 0 6	123.56	
.8490	5	1 3 4	130.28	
.8462	4	6 0 0	131.10	
.8447	2	2 1 6	131.53	
.8285	2	4 3 0	136.79	
.8202	7	0 4 0	139.80	
.8196	8	4 3 1	140.07	
.8194	2	6 1 0	140.15	
.8107	6	6 1 1	143.68	
.8107	3	3 2 5	143.68	
.8098	2	6 0 2	144.05	
.7967	2	5 1 4	150.40	
.7943	2	4 3 2	151.75	
.7917	11	3 1 6	153.28	
.7885	2	1 0 7	155.36	
.7870	2	0 4 2	156.33	
.7862	1	6 1 2	156.89	
.7833	13	5 2 3	159.09	

Cobalt phosphide, CoP_3

Structure

Cubic, $\text{Im}\bar{3}$ (204), $Z = 8$, isostructural with CoAs_3 , from powder data [Rundqvist and Ersson, 1968]. Munson and Kasper [1968] reported a high pressure phase deficient in cobalt, with a similar cell.

Atom positions [Rundqvist and Ersson, 1968]

8(c) 8 cobalt
24(g) 24 phosphorus

Lattice constant

$a = 7.7078 \text{ \AA}$
(published value, 7.7073 \AA [Rundqvist and Ersson, 1968]).

Volume

457.92 \AA^3

Density

(calculated) 4.404 g/cm^3

Thermal parameters

Isotropic [Rundqvist and Ersson, 1968].

Scattering factors

Co^0 , P^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)

$\gamma = 0.196 \times 10^{-3}$

References

- Cromer, D. T. and Mann, J. B. (1968). Acta Cryst-allogr. A24, 321.
Munson, R. A. and Kasper, J. S. (1968). Inorg. Chem. 7, 390.
Rundqvist, S. and Ersson, N. (1968). Ark. Kemi 30, 103.

Calculated Pattern (Peak heights)

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
5.447	25	1 1 0	16.26	
3.8538	100	2 0 0	23.06	
3.1467	15	2 1 1	28.34	
2.7250	65	2 2 0	32.84	
2.4365	100	0 1 3	36.86	
2.2245	30	2 2 2	40.52	
2.0598	25	1 2 3	43.92	
1.9271	8	4 0 0	47.12	
1.8166	6	3 3 0+	50.18	
1.7233	90	4 2 0+	53.10	
1.6435	6	3 3 2	55.90	
1.5735	50	4 2 2	58.62	
1.5115	25	4 3 1+	61.28	
1.3624	2	4 4 0	68.86	
1.3220	7	4 3 3+	71.28	
1.2847	2	4 4 2	73.68	
1.2188	13	0 2 6+	78.40	
1.1892	1	1 4 5+	80.74	
1.1620	11	6 2 2	83.04	
1.1365	7	1 3 6	85.34	
1.1125	10	4 4 4	87.64	
1.0901	2	3 4 5+	89.92	
1.0689	11	6 4 0+	92.22	
1.0488	3	6 3 3+	94.52	
1.0299	5	2 4 6+	96.82	
1.0121	6	7 3 0	99.12	
.9789	4	2 3 7+	103.80	
.9635	4	8 0 0	106.16	
.9488	1	1 4 7+	108.56	
.9347	11	6 4 4+	111.00	
.9213	1	3 5 6+	113.46	
.9084	12	6 6 0+	115.98	
.8960	11	7 4 3+	118.56	
.8842	3	6 6 2	121.20	
.8618	1	8 4 0+	126.72	
.8512	2	0 1 9+	129.64	
.8410	7	2 4 8+	132.68	
.8311	1	7 6 1+	135.88	
.8216	1	6 6 4	139.28	
.8125	1	4 5 7+	142.92	
.7950	6	3 6 7+	151.36	
.7867	4	8 4 4	156.58	

Cobalt phosphide, CoP_3 -(continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{Å}$
5.450	20	1 1 0	16.25	
3.8539	100	2 0 0	23.06	
3.1467	16	2 1 1	28.34	
2.7251	70	2 2 0	32.84	
2.4374	18	3 1 0	36.85	
2.4374	95	0 1 3	36.85	
2.2251	35	2 2 2	40.51	
2.0600	25	1 2 3	43.92	
1.9270	10	4 0 0	47.13	
1.8167	5	3 3 0	50.17	
1.8167	2	4 1 1	50.17	
1.7235	60	4 2 0	53.09	
1.7235	50	0 2 4	53.09	
1.6433	7	3 3 2	55.91	
1.5733	60	4 2 2	58.63	
1.5116	25	4 3 1	61.27	
1.5116	2	5 1 0	61.27	
1.5116	2	0 1 5	61.27	
1.5116	5	1 3 4	61.27	
1.3626	3	4 4 0	68.85	
1.3219	2	5 3 0	71.29	
1.3219	5	4 3 3	71.29	
1.3219	3	0 3 5	71.29	
1.2846	3	4 4 2	73.69	
1.2187	8	6 2 0	78.40	
1.2187	9	0 2 6	78.40	
1.1893	1	1 4 5	80.73	
1.1620	15	6 2 2	83.04	
1.1365	1	6 3 1	85.35	
1.1365	8	1 3 6	85.35	
1.1125	13	4 4 4	87.64	
1.0900	1	5 4 3	89.93	
1.0900	1	0 1 7	89.93	
1.0900	1	3 4 5	89.93	
1.0689	8	6 4 0	92.22	
1.0689	7	0 4 6	92.22	
1.0489	2	6 3 3	94.51	
1.0489	1	1 2 7	94.51	
1.0300	2	6 4 2	96.81	
1.0300	4	2 4 6	96.81	
1.0121	8	7 3 0	99.12	
1.0121	1	0 3 7	99.12	
.9789	4	2 3 7	103.80	
.9635	6	8 0 0	106.16	
.9488	1	1 4 7	108.56	
.9347	2	8 2 0	111.00	
.9347	4	0 2 8	111.00	
.9347	10	6 4 4	111.00	
.9213	2	3 5 6	113.47	
.9084	14	6 6 0	115.99	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{Å}$
.9084	5	8 2 2	115.99	
.8960	1	0 5 7	118.56	
.8960	1	7 5 0	118.56	
.8960	2	1 3 8	118.56	
.8960	11	7 4 3	118.56	
.8960	1	3 4 7	118.56	
.8841	5	6 6 2	121.21	
.8618	2	8 4 0	126.73	
.8512	2	0 1 9	129.64	
.8410	8	8 4 2	132.68	
.8410	8	2 4 8	132.68	
.8312	1	7 6 1	135.88	
.8312	1	1 2 9	135.88	
.8217	3	6 6 4	139.27	
.8125	1	7 5 4	142.92	
.8125	2	4 5 7	142.92	
.7950	2	9 3 2	151.36	
.7950	16	3 6 7	151.36	
.7867	12	8 4 4	156.58	

Cobalt plutonium, CoPu₂

Structure

Hexagonal, $P\bar{6}2m$ (189), $Z = 3$, cobalt-rich end member, isostructural with Fe₂P, from powder data [Ellinger, 1961].

Atom positions

The positions were assigned by comparisons of cell edge and atomic radii ratios; the positions for Ni₆Si₂P [Rundqvist and Jellinek, 1959] were preferred to those for Fe₂P, for this cobalt-rich end member.

3(f) 3 plutonium 2(c) 2 cobalt
3(g) 3 plutonium 1(b) 1 cobalt

Lattice constants [Ellinger, 1961]

$a = 7.763 \text{ \AA}$
 $c = 3.648$

Volume

190.4 \AA^3

Density

(calculated) 14.21 g/cm^3

Thermal parameters

Isotropic: plutonium, $B = 0.4$
cobalt, $B = 0.52$, the value for nickel,
used by Rundqvist and Jellinek [1959].

Scattering factors

Co⁰, Pu⁰ [International Tables, 1962], corrected for anomalous dispersion [Dauben and Templeton, 1955].

Scale factor (integrated intensities)

$\gamma = 0.707 \times 10^{-3}$

References

- Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. **8**, 241.
Ellinger, F. H. (1961). The Metal Plutonium. World Metallurgical Congress, 1957 (Univ. of Chicago Press, Chicago) p. 288.
International Tables for X-ray Crystallography, **III** (1962). (The Kynoch Press, Birmingham, England) pp. 204, 212.
Rundqvist, S. and Jellinek, F. (1959). Acta Chem. Scand. **13**, 425.

Calculated Pattern (Peak heights)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
6.72	7	1 0 0	13.16	
3.880	16	1 1 0	22.90	
3.361	1	2 0 0	26.50	
3.207	9	1 0 1	27.80	
2.657	100	1 1 1	33.70	
2.541	60	2 1 0	35.30	
2.472	40	2 0 1	36.32	
2.240	20	3 0 0	40.22	
2.085	15	2 1 1	43.36	
1.940	3	2 2 0	46.78	
1.910	1	3 0 1	47.58	
1.865	6	3 1 0	48.80	
1.824	12	0 0 2	49.96	
1.713	2	2 2 1	53.44	
1.681	3	4 0 0	54.56	
1.660	15	3 1 1	55.28	
1.651	3	1 1 2	55.62	
1.542	4	3 2 0	59.92	
1.526	8	4 0 1	60.62	
1.482	17	2 1 2	62.64	
1.467	2	4 1 0	63.34	
1.420	16	3 2 1	65.68	
1.415	10	3 0 2	65.98	
1.361	5	4 1 1	68.94	
1.345	4	5 0 0	69.90	
1.329	2	2 2 2	70.84	
1.304	3	3 1 2	72.42	
1.294	2	3 3 0	73.08	
1.271	4	4 2 0	74.64	
1.262	2	5 0 1	75.26	
1.236	2	4 0 2	77.10	
1.219	1	3 3 1	78.36	
1.207	2	5 1 0	79.28	
1.200	4	4 2 1	79.88	
1.178	3	3 2 2	81.70	
1.160	5	1 1 3	83.18	
1.146	2	5 1 1	84.44	
1.143	4	2 0 3+	84.70	
1.097	1	2 1 3	89.22	
1.082	4	5 0 2	90.76	
1.076	1	5 2 0	91.38	
1.058	1	4 3 1	93.48	
1.055	3	3 3 2	93.76	
1.042	4	4 2 2	95.28	
1.032	3	5 2 1	96.50	
1.025	1	6 1 0	97.42	
1.018	3	3 1 3	98.28	
1.007	3	5 1 2	99.82	
.987	8	6 1 1	102.60	
.985	5	4 0 3	102.96	

Cobalt plutonium, CoPu₂ - (continued)

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
.970	1	4 4 0	105.08	
.960	2	5 3 0	106.66	
.955	5	3 2 3	107.54	
.945	1	4 3 2	109.16	
.938	4	4 4 1	110.46	
.936	2	4 1 3	110.74	
.929	1	5 3 1	112.08	
.927	2	5 2 2	112.38	
.912	1	0 0 4	115.26	
.903	1	6 2 1	117.04	
.902	1	5 0 3	117.32	
.894	2	6 1 2	119.06	
.891	1	7 1 0	119.76	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
1.236	2	4 0 2	77.10	
1.219	1	3 3 1	78.35	
1.207	3	5 1 0	79.28	
1.200	4	4 2 1	79.88	
1.178	4	3 2 2	81.70	
1.160	6	1 1 3	83.18	
1.146	2	5 1 1	84.44	
1.143	3	2 0 3	84.70	
1.143	1	4 1 2	84.73	
1.105	1	4 3 0	88.37	
1.097	2	2 1 3	89.22	
1.082	5	5 0 2	90.75	
1.077	2	5 2 0	91.37	
1.058	1	4 3 1	93.48	
1.055	3	3 3 2	93.76	
1.043	5	4 2 2	95.27	
1.033	4	5 2 1	96.50	
1.025	2	6 1 0	97.41	
1.019	4	3 1 3	98.27	
1.007	4	5 1 2	99.82	
.987	10	6 1 1	102.60	
.985	3	4 0 3	102.87	
.970	1	4 4 0	105.09	
.960	2	5 3 0	106.65	
.955	6	3 2 3	107.54	
.945	1	4 3 2	109.16	
.938	5	4 4 1	110.45	
.936	2	4 1 3	110.73	
.929	1	5 3 1	112.07	
.927	3	5 2 2	112.38	
.912	2	0 0 4	115.26	
.903	2	6 2 1	117.03	
.902	1	5 0 3	117.32	
.894	3	6 1 2	119.06	
.890	1	7 1 0	119.77	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
6.72	6	1 0 0	13.16	
3.882	15	1 1 0	22.89	
3.361	1	2 0 0	26.49	
3.206	9	1 0 1	27.80	
2.658	100	1 1 1	33.69	
2.541	60	2 1 0	35.29	
2.472	40	2 0 1	36.31	
2.241	25	3 0 0	40.21	
2.085	16	2 1 1	43.36	
1.941	3	2 2 0	46.77	
1.909	1	3 0 1	47.58	
1.865	7	3 1 0	48.80	
1.824	14	0 0 2	49.96	
1.713	3	2 2 1	53.43	
1.681	3	4 0 0	54.56	
1.660	17	3 1 1	55.28	
1.651	3	1 1 2	55.63	
1.542	5	3 2 0	59.92	
1.527	10	4 0 1	60.61	
1.482	20	2 1 2	62.64	
1.467	1	4 1 0	63.34	
1.421	19	3 2 1	65.67	
1.415	9	3 0 2	65.98	
1.361	6	4 1 1	68.93	
1.345	5	5 0 0	69.90	
1.329	2	2 2 2	70.84	
1.304	4	3 1 2	72.42	
1.294	2	3 3 0	73.08	
1.271	5	4 2 0	74.64	
1.262	2	5 0 1	75.26	

Cobalt plutonium, CoPu₆

Structure

Tetragonal, I4/mcm (140), Z = 4, isostructural with MnU₆, from powder data [Ellinger, 1961].

Atom positions

The positions and distributions of MnU₆ were used [Baenziger et al., 1950]

Lattice constants

[Poole et al., 1961, Table 6.1]

a = 10.476 Å

c = 5.340 Å

(published values: a = 10.475, c = 5.340 Å)

Volume

586.1 Å³

Density

(calculated) 17.12 g/cm³

Thermal parameters

Isotropic: cobalt, B = 1.0; plutonium, B = 0.75

Scattering factors

Co⁰, Pu⁰ [International Tables, 1962]

Scale factors (integrated intensities)

γ = 2.67 x 10⁻³

References

Baenziger, N. C., Rundle, R. E., Snow, A. I., and Wilson, A. S. (1950). Acta Crystallogr. 3, 34.

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Poole, D.M., Bale, M. G., Mardon, P. G., Marples, J. A. C., and Nichols, J. C. (1961). Plutonium 1960. International Conference on Plutonium Metallurgy, (2nd). Cleaver Hume Press, London). p. 276.

Calculated Pattern (Peak heights)

d(Å)	I	hkl	2θ(°) λ = 1.540598Å
7.41	4	1 1 0	11.94
3.70	1	2 2 0	24.02
3.52	2	2 1 1	25.28
3.31	2	3 1 0	26.90
2.670	30	0 0 2	33.54
2.618	5	4 0 0	34.22
2.552	100	3 2 1	35.14
2.512	4	1 1 2	35.72
2.469	2	3 3 0	36.36
2.378	1	2 0 2	37.80
2.342	6	4 2 0	38.40
2.294	6	4 1 1	39.24
2.166	2	2 2 2	41.66
2.079	4	3 1 2	43.50
2.055	12	5 1 0	44.04
1.951	2	4 3 1	46.52
1.870	5	4 0 2	48.66
1.761	2	4 2 2	51.88
1.746	5	6 0 0	52.36
1.639	6	6 1 1	56.06
1.628	7	5 1 2	56.48
1.518	17	3 2 3	61.00
1.481	6	5 5 0	62.66
1.461	7	6 0 2	63.62
1.458	5	4 1 3	63.80
1.389	4	7 2 1	67.34
1.335	3	0 0 4	70.48
1.295	9	5 5 2	72.98
1.238	2	6 1 3	76.98
1.235	2	6 6 0	77.20
1.195	11	8 3 1	80.28
1.160	1	4 2 4	83.24
1.119	4	5 1 4+	86.98
1.111	1	7 6 1+	87.76
1.061	2	6 0 4	93.16
1.048	2	10 0 0	94.66
1.021	1	9 3 2	98.02
1.010	7	8 3 3	99.44
1.002	4	3 2 5	100.42
.992	3	5 5 4	101.92
.975	3	10 0 2	104.34
.969	3	8 7 1	105.28
.958	1	7 6 3+	107.08

Cobalt plutonium, CoPu₆ - (continued)

Calculated Pattern (Integrated)					
d(Å)	I	hkl			2θ(°) λ = 1.540598Å
7.41	3	1	1	0	11.94
3.70	1	2	2	0	24.01
3.52	2	2	1	1	25.27
3.31	2	3	1	0	26.89
2.670	25	0	0	2	33.54
2.619	4	4	0	0	34.21
2.552	100	3	2	1	35.13
2.512	2	1	1	2	35.72
2.469	2	3	3	0	36.35
2.379	1	2	0	2	37.79
2.343	6	4	2	0	38.40
2.294	6	4	1	1	39.24
2.166	2	2	2	2	41.67
2.079	4	3	1	2	43.50
2.055	13	5	1	0	44.04
1.950	2	4	3	1	46.52
1.870	5	4	0	2	48.66
1.761	2	4	2	2	51.88
1.746	6	6	0	0	52.36
1.639	6	6	1	1	56.06
1.628	8	5	1	2	56.47
1.522	1	4	4	2	60.82
1.518	19	3	2	3	61.00
1.482	7	5	5	0	62.66
1.461	8	6	0	2	63.62
1.458	1	4	1	3	63.79
1.389	5	7	2	1	67.34
1.335	3	0	0	4	70.48
1.295	10	5	5	2	72.97
1.238	2	6	1	3	76.98
1.235	1	6	6	0	77.21
1.195	13	8	3	1	80.27
1.160	1	4	2	4	83.23
1.121	1	6	6	2	86.85
1.119	3	5	1	4	86.96
1.119	2	7	2	3	87.00
1.061	2	6	0	4	93.16
1.048	2	10	0	0	94.66
1.020	1	9	3	2	98.03
1.010	8	8	3	3	99.43
1.002	5	3	2	5	100.43
.992	4	5	5	4	101.92
.975	3	10	0	2	104.35
.969	4	8	7	1	105.28

Cobalt plutonium, Co₂Pu

Structure

Cubic, Fd3m (227), Z = 8, isostructural with Cu₂Mg, from powder data [Ellinger, 1961]. Their sample was described as plutonium-rich.

Atom positions

8(a) 8 plutonium
16(d) 16 cobalt
The origin was taken at $\bar{4}3m$.

Lattice constant

a = 7.081 Å [Ellinger, 1961].

Volume

355.1 Å³

Density

(calculated) 13.462 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co⁰ [Cromer and Mann, 1968]
Pu⁰ [International Tables, 1974]

Scale factor (integrated intensities)

$\gamma = 1.370 \times 10^{-3}$

References

- Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.
Ellinger, F. H. (1961). In The Metal Plutonium, (Univ. of Chicago Press, Chicago). World Metallurgical Conference, 1957 (edited by Coffinberry, A. S. and Miner, W. N.) p. 288.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.

Calculated Pattern (Peak heights)

d (Å)	I	hkl	2θ (°)
$\lambda = 1.540598\text{Å}$			
4.08	45	1 1 1	21.74
2.504	90	2 2 0	35.84
2.135	100	3 1 1	42.30
2.044	10	2 2 2	44.28
1.771	5	4 0 0	51.58
1.624	10	3 3 1	56.62
1.446	25	4 2 2	64.40
1.363	25	5 1 1+	68.84
1.252	15	4 4 0	75.96
1.197	5	5 3 1	80.12
1.120	10	6 2 0	86.94
1.080	5	5 3 3	91.02
1.067	1	6 2 2	92.38
1.022	1	4 4 4	97.82
.991	5	7 1 1+	101.96
.946	10	6 4 2	109.00
.922	15	7 3 1+	113.36
.885	5	8 0 0	120.98
.865	1	7 3 3	125.86
.834	5	8 2 2+	134.76

Calculated Pattern (Integrated)

d (Å)	I	hkl	2θ (°)
$\lambda = 1.540598\text{Å}$			
4.09	40	1 1 1	21.72
2.504	85	2 2 0	35.84
2.135	100	3 1 1	42.30
2.044	10	2 2 2	44.28
1.770	5	4 0 0	51.59
1.624	10	3 3 1	56.61
1.445	30	4 2 2	64.41
1.363	20	5 1 1	68.84
1.363	5	3 3 3	68.84
1.252	20	4 4 0	75.96
1.197	5	5 3 1	80.12
1.120	10	6 2 0	86.95
1.080	10	5 3 3	91.02
1.068	1	6 2 2	92.37
1.022	1	4 4 4	97.82
.992	1	7 1 1	101.95
.992	1	5 5 1	101.95
.946	15	6 4 2	108.99
.922	15	7 3 1	113.35
.922	5	5 5 3	113.35
.885	5	8 0 0	120.98
.865	1	7 3 3	125.86
.835	10	8 2 2	134.76
.835	5	6 6 0	134.76
.818	15	7 5 1	140.81

Cobalt plutonium, Co₃Pu

Structure

Hexagonal, $R\bar{3}m$ (166), $Z = 9$, isostructural with Ni_3Pu , from powder data [Poole et al., 1961].

Atom positions

The positions assumed were those refined for Ni_3Pu [Cromer and Olsen, 1959].

Lattice constants [Poole et al., 1961]

$a = 5.003 \text{ \AA}$

$c = 24.42$

Volume

529.3 \AA^3

Density

(calculated) 11.82 g/cm^3

Thermal parameters

Isotropic values were used from Cromer and Olsen [1959], with their data for nickel applied to the cobalt atoms here.

Scattering factors

Co^0 , Pu^0 [International Tables, 1962], corrected for anomalous dispersion [Cromer and Olsen, 1959].

Scale factor (integrated intensities)

$\gamma = 0.369 \times 10^{-3}$

References

Cromer, D. T. and Olsen, C. E. (1959). Acta Cryst-allogr. 12, 689.

International Tables for X-ray Crystallography, III, (The Kynoch Press, Birmingham, England), pp. 202,204.

Poole, D. M., Bale, M. G., Marden, P. G., Marples, J. A. C., and Nichols, J. L. (1961). In Plutonium, 1960 (Cleaver Hume Press, London). International Conference on Plutonium Metallurgy, (2nd). Edited by Grison, E., Lord, W. B. H., and Fowler, R. D., p. 267.

Calculated Pattern (Peak heights)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
8.14	8	0 0 3	10.86	
4.26	35	1 0 1	20.82	
4.07	14	0 0 6	21.82	
3.531	5	1 0 4	25.20	
3.241	2	0 1 5	27.50	
2.717	65	1 0 7	32.94	
2.501	80	1 1 0	35.88	
2.495	85	0 1 8	35.96	
2.391	2	1 1 3	37.58	
2.157	35	0 2 1	41.84	
2.131	100	1 1 6	42.38	
2.041	10	0 2 4	44.34	
2.035	13	0 0 12	44.48	
1.975	14	0 1 11+	45.90	
1.839	6	1 1 9+	49.52	
1.767	4	2 0 8	51.70	
1.723	2	1 0 13	53.10	
1.634	4	2 1 1	56.26	
1.628	5	0 0 15	56.48	
1.618	10	0 1 14	56.86	
1.581	1	2 1 4	58.30	
1.578	2	1 1 12	58.42	
1.482	15	2 1 7	62.62	
1.444	17	1 2 8+	64.50	
1.419	7	0 2 13	65.74	
1.364	12	1 1 15	68.74	
1.361	25	3 0 6+	68.94	
1.359	18	2 0 14	69.08	
1.318	4	1 2 11	71.54	
1.2749	1	0 3 9+	74.34	
1.2506	13	2 2 0	76.04	
1.2344	1	2 1 13	77.22	
1.2001	2	1 3 1	79.86	
1.1971	4	2 0 17	80.10	
1.1939	8	1 2 14	80.36	
1.1753	2	0 1 20	81.90	
1.1630	1	0 0 21	82.96	
1.1361	6	1 3 7	85.38	
1.1182	4	3 1 8	87.08	
1.1154	3	2 1 16	87.36	
1.1053	1	0 2 19	88.36	
1.0820	3	4 0 1	90.78	
1.0804	5	3 0 15+	90.96	
1.0754	2	1 0 22	91.50	
1.0656	4	2 2 12	92.58	
1.0569	2	3 1 11	93.58	
1.0545	7	1 1 21	93.86	
1.0208	1	0 4 8	97.98	

Cobalt plutonium, Co₃Pu - (continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
8.14	7	0 0 3	10.86	
4.27	30	1 0 1	20.81	
4.08	2	0 1 2	21.75	
4.07	12	0 0 6	21.82	
3.533	4	1 0 4	25.18	
3.241	2	0 1 5	27.50	
2.717	65	1 0 7	32.94	
2.713	3	0 0 9	32.99	
2.502	70	1 1 0	35.87	
2.495	45	0 1 8	35.96	
2.391	2	1 1 3	37.59	
2.158	40	0 2 1	41.83	
2.133	8	2 0 2	42.34	
2.131	100	1 1 6	42.38	
2.127	4	1 0 10	42.46	
2.042	9	0 2 4	44.33	
2.035	10	0 0 12	44.48	
1.980	8	2 0 5	45.78	
1.976	11	0 1 11	45.89	
1.840	2	0 2 7	49.49	
1.839	5	1 1 9	49.52	
1.767	4	2 0 8	51.70	
1.723	2	1 0 13	53.10	
1.634	4	2 1 1	56.25	
1.628	4	0 0 15	56.48	
1.618	11	0 1 14	56.86	
1.582	1	2 1 4	58.29	
1.579	1	1 1 12	58.41	
1.482	18	2 1 7	62.61	
1.444	11	3 0 0	64.47	
1.443	14	1 2 8	64.52	
1.440	1	1 0 16	64.70	
1.419	8	0 2 13	65.74	
1.364	12	1 1 15	68.74	
1.361	10	0 3 6	68.94	
1.361	10	3 0 6	68.94	
1.360	1	2 1 10	68.99	
1.359	12	2 0 14	69.08	
1.318	5	1 2 11	71.54	
1.2508	17	2 2 0	76.03	
1.2344	1	2 1 13	77.22	
1.2002	2	1 3 1	79.85	
1.1972	3	2 0 17	80.09	
1.1956	2	2 2 6	80.23	
1.1939	7	1 2 14	80.36	
1.1752	2	0 1 20	81.91	
1.1629	2	0 0 21	82.97	
1.1362	7	1 3 7	85.37	
1.1359	1	2 2 9	85.40	
1.1182	6	3 1 8	87.09	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
1.1165	1	2 1 16	87.25	
1.1054	1	0 2 19	88.35	
1.0821	3	4 0 1	90.77	
1.0804	3	3 0 15	90.96	
1.0804	3	0 3 15	90.96	
1.0753	2	1 0 22	91.51	
1.0665	1	4 0 4	92.48	
1.0656	5	2 2 12	92.59	
1.0568	2	3 1 11	93.59	
1.0545	8	1 1 21	93.86	
1.0208	1	0 4 8	97.98	
1.0123	1	1 3 13	99.10	

Cobalt plutonium, Co₁₇Pu₂

Structure

Hexagonal, P6₃/mmc (194), Z = 2, isostructural with Ni₁₇Th₂, from powder data [Ellinger, 1961]. Bouchet et al. [1966] determined positions for Co₁₇Ho₂, a similar isostructural compound.

Atom positions

From considerations of atomic size, the positions for Co₁₇Ho₂ were used.

6(g) 6 cobalt(1)
12(j) 12 cobalt(2)
12(k) 12 cobalt(3)
4(f) 4 cobalt(4)
2(b) 2 plutonium(1)
2(d) 2 plutonium(2)

Lattice constants

a = 8.325 Å
c = 8.104 [Ellinger, 1961]

Volume
486.4 Å³

Density

(calculated) 10.145 g/cm³

Thermal parameters

Isotropic: cobalt B = 0.6; plutonium B = 0.5.

Scattering factors

Co⁰ [International Tables, 1962]
Pu⁰ [International Tables, 1974]

Scale factor (integrated intensities)

$\gamma = 0.399 \times 10^{-3}$

References

- Bouchet, G., Laforest, J., Lemaire, R., and Schweizer, J. (1966). C. R. Acad. Sci. Ser. B, 262, 1227.
Ellinger, F. H. (1961). In The Metal Plutonium (Univ. of Chicago Press, Chicago). World Metallurgical Conference, 1957 (edited by Coffinberry, A. S. and Miner, W. N.) p. 288.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 204.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.

Calculated Pattern (Peak heights)

d(Å)	I	hkl	2θ(°) λ = 1.540598Å
7.202	1	1 0 0	12.28
5.381	16	1 0 1	16.46
4.160	19	1 1 0	21.34
4.052	8	0 0 2	21.92
3.604	2	2 0 0	24.68
3.531	6	1 0 2	25.20
3.293	12	2 0 1	27.06
2.903	60	1 1 2	30.78
2.725	2	2 1 0	32.84
2.693	7	2 0 2	33.24
2.583	13	2 1 1	34.70
2.529	11	1 0 3	35.46
2.403	45	3 0 0	37.40
2.261	6	2 1 2	39.84
2.161	25	2 0 3	41.76
2.081	55	2 2 0	43.44
2.067	100	3 0 2	43.76
2.026	25	0 0 4	44.70
1.951	2	1 0 4	46.52
1.942	1	3 1 1	46.74
1.919	14	2 1 3	47.34
1.851	4	2 2 2	49.18
1.793	1	3 1 2	50.88
1.766	3	2 0 4	51.72
1.626	4	2 1 4	56.56
1.621	7	3 2 1	56.76
1.607	3	3 1 3	57.28
1.581	3	1 0 5	58.30
1.573	4	4 1 0	58.64
1.549	10	3 0 4	59.64
1.531	3	3 2 2	60.40
1.499	2	4 0 3	61.84
1.478	1	2 0 5	62.82
1.467	15	4 1 2	63.36
1.452	15	2 2 4	64.10
1.423	1	3 1 4	65.54
1.420	2	5 0 1	65.72
1.411	7	3 2 3	66.20
1.393	5	2 1 5	67.14
1.388	6	3 3 0	67.44
1.359	1	5 0 2	69.08
1.351	1	0 0 6	69.54
1.344	1	4 2 1	69.96
1.313	15	3 3 2	71.86
1.291	1	4 2 2	73.24
1.285	6	1 1 6	73.68
1.281	5	3 2 4	73.90
1.278	3	5 1 1	74.10
1.272	3	5 0 3	74.54
1.259	1	3 1 5	75.44

Cobalt plutonium, Co₁₇Pu₂ - (Continued)

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
1.233	1	5 1 2	77.30	
1.216	5	4 2 3	78.58	
1.202	12	6 0 0	79.74	
1.177	13	3 0 6	81.72	
1.168	3	5 1 3	82.56	
1.158	4	3 2 5	83.42	
1.155	3	5 2 0	83.70	
1.145	3	3 3 4	84.58	
1.131	1	4 2 4	85.90	
1.110	6	5 2 2	87.86	
1.102	1	2 0 7	88.66	
1.091	1	5 1 4	89.82	
1.077	1	5 0 5	91.30	
1.041	5	4 4 0	95.50	
1.033	10	6 0 4	96.38	
1.025	6	4 1 6	97.46	
1.018	1	6 1 3	98.28	
1.013	3	0 0 8	99.00	
1.012	3	5 1 5	99.18	
.992	1	6 2 1	101.84	
.984	1	1 1 8	103.00	
.971	1	6 2 2	105.04	
.968	7	3 3 6	105.48	
.962	2	5 3 3	106.34	
.955	1	7 1 0	107.54	
.938	4	6 2 3	110.48	
.933	4	3 0 8	111.22	
.929	5	7 1 2	111.94	
.926	5	4 4 4	112.64	
.918	1	5 3 4	114.08	
.917	1	5 4 1	114.24	
.911	5	2 2 8	115.50	
.908	4	6 3 0	115.98	
.898	1	6 0 6	118.20	
.897	1	6 2 4	118.44	
.894	1	1 0 9	119.10	
.886	8	6 3 2	120.70	
.882	2	4 2 7	121.64	
.878	5	5 2 6	122.74	
.873	2	5 4 3	123.74	
.869	2	5 3 5	124.78	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
7.210	1	1 0 0	12.27	
5.387	13	1 0 1	16.44	
4.163	17	1 1 0	21.33	
4.052	7	0 0 2	21.92	
3.605	2	2 0 0	24.68	
3.532	6	1 0 2	25.19	
3.294	11	2 0 1	27.05	
2.903	60	1 1 2	30.77	
2.725	1	2 1 0	32.84	
2.693	6	2 0 2	33.24	
2.583	13	2 1 1	34.70	
2.530	11	1 0 3	35.46	
2.403	45	3 0 0	37.39	
2.261	6	2 1 2	39.83	
2.162	25	2 0 3	41.75	
2.081	55	2 2 0	43.45	
2.067	100	3 0 2	43.76	
2.026	25	0 0 4	44.69	
1.950	2	1 0 4	46.52	
1.941	1	3 1 1	46.75	
1.918	15	2 1 3	47.35	
1.851	5	2 2 2	49.17	
1.793	1	3 1 2	50.88	
1.766	3	2 0 4	51.72	
1.654	1	3 2 0	55.51	
1.626	3	2 1 4	56.56	
1.621	6	3 2 1	56.76	
1.607	3	3 1 3	57.28	
1.581	3	1 0 5	58.30	
1.573	4	4 1 0	58.63	
1.549	11	3 0 4	59.64	
1.531	3	3 2 2	60.40	
1.499	2	4 0 3	61.83	
1.478	1	2 0 5	62.81	
1.467	17	4 1 2	63.37	
1.452	17	2 2 4	64.09	
1.423	1	3 1 4	65.54	
1.420	2	5 0 1	65.72	
1.411	8	3 2 3	66.20	
1.393	5	2 1 5	67.14	
1.388	6	3 3 0	67.44	
1.358	1	5 0 2	69.09	
1.351	1	0 0 6	69.54	
1.344	1	4 2 1	69.96	
1.313	17	3 3 2	71.86	
1.291	1	4 2 2	73.23	
1.285	6	1 1 6	73.68	
1.281	2	3 2 4	73.91	
1.279	3	5 1 1	74.09	
1.272	3	5 0 3	74.54	

Cobalt plutonium, Co₁₇Pu₂ - (Continued)

Calculated Pattern (Integrated)					
d(Å)	I	hkl			2θ(°) λ = 1.540598Å
1.259	2	3	1	5	75.44
1.233	1	5	1	2	77.29
1.217	5	4	2	3	78.57
1.202	14	6	0	0	79.74
1.177	16	3	0	6	81.72
1.175	1	5	0	4	81.95
1.168	4	5	1	3	82.55
1.158	4	3	2	5	83.43
1.154	2	5	2	0	83.71
1.145	3	3	3	4	84.58
1.131	1	4	2	4	85.89
1.110	7	5	2	2	87.86
1.102	2	2	0	7	88.67
1.091	1	5	1	4	89.82
1.077	2	5	0	5	91.29
1.041	6	4	4	0	95.50
1.034	12	6	0	4	96.37
1.025	8	4	1	6	97.47
1.022	1	5	3	1	97.86
1.018	1	6	1	3	98.30
1.013	3	0	0	8	99.00
1.012	3	5	1	5	99.18
.998	1	5	3	2	101.01
.992	1	6	2	1	101.85
.984	1	1	1	8	103.00
.971	1	6	2	2	105.04
.968	8	3	3	6	105.48
.962	3	5	3	3	106.34
.955	2	7	1	0	107.54
.938	5	6	2	3	110.48
.933	5	3	0	8	111.22
.929	7	7	1	2	111.94
.926	7	4	4	4	112.64
.918	1	5	3	4	114.07
.917	1	5	4	1	114.25
.911	7	2	2	8	115.49
.910	1	6	1	5	115.69
.908	3	6	3	0	116.00
.898	1	6	0	6	118.19
.897	1	6	2	4	118.44
.894	1	1	0	9	119.11
.886	11	6	3	2	120.70
.882	2	4	2	7	121.65
.878	7	5	2	6	122.75
.876	1	7	2	1	123.21
.874	3	5	4	3	123.73
.869	3	5	3	5	124.78

Cobalt praseodymium, Co₂Pr

Structure

Cubic, Fd3m (227), Z = 8, isostructural with Cu₂Mg, from powder data [Harris et al., 1965].

Atom positions

8(a) 8 praseodymium
16(d) 16 cobalt

Lattice constant

a = 7.3063 Å
(published value, 7.2911 kX [Harris et al., 1965]).

Volume

390.0 Å³

Density

(calculated) 8.814 g/cm³

Thermal parameters

Isotropic: overall B = 1.0

Scattering factors

Co⁰ [Cromer and Mann, 1968]
Pr⁰ [International Tables, 1974]

Scale factor (integrated intensities)

γ = 0.575 × 10⁻³

References

- Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.
Harris, I. R., Mansey, R. C., and Raynor, G. V. (1965). J. Less-Common Metals 9, 270.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 100.

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
4.215	10	1 1 1	21.06	
2.583	65	2 2 0	34.70	
2.203	100	3 1 1	40.94	
2.109	15	2 2 2	42.84	
1.676	1	3 3 1	54.72	
1.4913	15	4 2 2	62.20	
1.4060	25	5 1 1+	66.44	
1.2917	15	4 4 0	73.22	
1.2350	1	5 3 1	77.18	
1.1552	5	6 2 0	83.64	
1.1141	5	5 3 3	87.48	
1.1015	5	6 2 2	88.74	
1.0231	1	7 1 1+	97.68	
.9763	5	6 4 2	104.18	
.9512	10	7 3 1+	108.16	
.9133	1	8 0 0	115.00	
.8610	5	8 2 2+	126.92	
.8437	10	7 5 1+	131.86	
.8381	1	6 6 2	133.60	
.8020	1	7 5 3+	147.68	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
4.218	10	1 1 1	21.04	
2.583	60	2 2 0	34.70	
2.203	100	3 1 1	40.93	
2.109	15	2 2 2	42.84	
1.676	1	3 3 1	54.72	
1.4914	20	4 2 2	62.20	
1.4061	20	5 1 1	66.44	
1.4061	5	3 3 3	66.44	
1.2916	20	4 4 0	73.22	
1.2350	1	5 3 1	77.18	
1.1552	5	6 2 0	83.64	
1.1142	10	5 3 3	87.47	
1.1015	5	6 2 2	88.75	
.9763	10	6 4 2	104.18	
.9512	10	7 3 1	108.16	
.9512	5	5 5 3	108.16	
.9133	5	8 0 0	115.01	
.8611	1	6 6 0	126.91	
.8611	5	8 2 2	126.91	
.8437	10	7 5 1	131.86	
.8437	1	5 5 5	131.86	
.8381	5	6 6 2	133.59	
.8020	1	7 5 3	147.69	
.8020	1	9 1 1	147.69	

Cobalt rhodium sulfide, Co_8RhS_8

Structure

Cubic, $\text{Fm}\bar{3}\text{m}$ (225), $Z = 4$, π phase, isostructural with Co_9S_8 , from powder data [Knop, 1962].

Atom positions [Pearson, 1967]

32(f) 32 cobalt 8(c) 8 sulfur
4(b) 4 rhodium 24(e) 24 sulfur

Lattice constant

$a = 9.978(2) \text{ \AA}$
(published value, $a = 9.977(2) \text{ \AA}$, [Knop, 1962])

Volume

993.4 \AA^3

Density

(calculated) 5.555 g/cm^3

Thermal parameters

Isotropic: cobalt, $B = 0.5$; rhodium, $B = 0.4$;
sulfur, $B = 0.7$

Scattering factors

Co^0 , Rh^0 , S^0 [International tables, 1962]

Scale factors (integrated intensities)

$\gamma = 0.413 \times 10^{-3}$

References

- International Tables for X-ray Crystallography III
(1962). (The Kynoch Press, Birmingham, England).
pp. 202, 204, 210.
Knop, D. (1962). Chem. Ind. London, April 21,
p. 739.
Pearson, W. B. (1967). Handbook of Lattice
Spacings and Structures of Metals and Alloys,
v.2, (Pergamon Press, N.Y.), pp. 204, 807.

Calculated Pattern (Peak heights)

$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.540598\text{\AA}$
5.757	7	1 1 1	15.38
4.985	12	2 0 0	17.78
3.526	12	2 2 0	25.24
3.008	100	3 1 1	29.68
2.881	10	2 2 2	31.02
2.494	3	4 0 0	35.98
2.288	5	3 3 1	39.34
2.231	7	4 2 0	40.40
2.037	4	4 2 2	44.44
1.920	30	5 1 1+	47.30
1.763	75	4 4 0	51.80
1.686	1	5 3 1	54.36
1.663	2	4 4 2+	55.18
1.577	2	6 2 0	58.46
1.522	9	5 3 3	60.82
1.504	2	6 2 2	61.60
1.3334	2	6 4 2	70.58
1.2990	14	7 3 1+	72.74
1.2473	9	8 0 0	76.28
1.2190	1	7 3 3	78.38
1.2100	1	6 4 4+	79.08
1.1760	1	8 2 2+	81.84
1.1521	7	7 5 1+	83.92
1.1446	1	6 6 2	84.60
1.0886	1	8 4 2	90.08
1.0460	5	9 3 1	94.86
1.0183	18	8 4 4	98.30
.9785	1	8 6 2+	103.86
.9646	6	9 5 1+	105.98
.9601	1	10 2 2+	106.70
.9264	1	10 4 0+	112.50
.8997	3	11 1 1+	117.78
.8819	7	8 8 0	121.72
.8463	4	9 7 3+	131.06
.8433	1	10 6 2	131.96
.8093	1	10 6 4+	144.28
.8015	6	9 7 5+	147.94
.7888	14	12 4 0	155.12
.7792	1	8 8 6+	162.70

Cobalt rhodium sulfide, Co_8RhS_8 -(continued)

Calculated Pattern (Integrated)					
$d(\text{\AA})$	I	hkl			$2\theta(^{\circ})$ $\lambda = 1.540598\text{\AA}$
5.761	6	1	1	1	15.37
4.989	11	2	0	0	17.76
3.528	11	2	2	0	25.22
3.008	100	3	1	1	29.67
2.880	10	2	2	2	31.02
2.494	3	4	0	0	35.97
2.289	5	3	3	1	39.33
2.231	7	4	2	0	40.39
2.037	4	4	2	2	44.44
1.920	30	5	1	1	47.30
1.920	8	3	3	3	47.30
1.764	85	4	4	0	51.79
1.687	1	5	3	1	54.35
1.663	1	6	0	0	55.19
1.663	2	4	4	2	55.19
1.578	2	6	2	0	58.45
1.522	11	5	3	3	60.83
1.504	2	6	2	2	61.61
1.4402	1	4	4	4	64.67
1.3972	1	7	1	1	66.91
1.3837	1	6	4	0	67.66
1.3334	2	6	4	2	70.58
1.2990	11	7	3	1	72.74
1.2990	7	5	5	3	72.74
1.2472	11	8	0	0	76.28
1.2190	1	7	3	3	78.38
1.2100	1	6	4	4	79.08
1.1522	8	7	5	1	83.91
1.1522	2	5	5	5	83.91
1.1446	1	6	6	2	84.60
1.0887	1	8	4	2	90.07
1.0460	7	9	3	1	94.86
1.0184	25	8	4	4	98.30
.9784	1	8	6	2	103.87
.9646	6	9	5	1	105.99
.9646	2	7	7	3	105.99
.9264	1	10	4	0	112.50
.9109	1	10	4	2	115.49
.8997	2	11	1	1	117.78
.8997	2	7	7	5	117.78
.8819	11	8	8	0	121.72
.8718	1	11	3	1	124.16
.8463	2	11	3	3	131.06
.8463	5	9	7	3	131.06
.8433	1	10	6	2	131.97
.8093	2	10	6	4	144.27
.8015	7	11	5	3	147.94
.8015	9	9	7	5	147.94
.7888	45	12	4	0	155.11
.7792	2	8	8	6	162.71
.7792	2	12	4	2	162.71

Cobalt ruthenium sulfide, Co₈RuS₈

Structure

Cubic, Fm3m (225), Z = 4, π phase, isostructural with Co₉S₈, from powder data [Knop, 1962].

Atom positions [Pearson, 1967].

32(f) 32 cobalt 8(c) 8 sulfur
4(b) 4 ruthenium 24(e) 24 sulfur

Lattice constant [Knop, 1962]

a = 9.945(2) Å
(published value, a = 9.944(2) Å)

Volume Å³
983.6 Å³

Density

(calculated) 5.599 g/cm³

Thermal parameters

Isotropic: cobalt, B = 0.5; ruthenium, B = 0.4;
sulfur, B = 0.7

Scattering factors

Co⁰, Ru⁰, S⁰ [International Tables, 1962]

Scale factors (integrated intensities)

$\gamma = 0.409 \times 10^{-3}$

References

- International Tables for X-ray Crystallography III
(1962). (The Kynoch Press, Birmingham, England)
pp. 202, 204, 210.
Knop, O. (1962). Chem. Ind. London, April 21,
p. 739.
Pearson, W.B. (1967). Handbook of Lattice Spacings
and Structures of Metals and Alloys, V.2, (Perg-
amon Press, N.Y.). pp. 204, 808.

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{Å}$
5.734	8	1 1 1	15.44	
4.968	12	2 0 0	17.84	
3.515	11	2 2 0	25.32	
2.998	100	3 1 1	29.78	
2.870	10	2 2 2	31.14	
2.486	3	4 0 0	36.10	
2.282	5	3 3 1	39.46	
2.223	6	4 2 0	40.54	
2.030	4	4 2 2	44.60	
1.9141	30	5 1 1+	47.46	
1.7578	75	4 4 0	51.98	
1.6812	1	5 3 1	54.54	
1.6577	2	4 4 2+	55.38	
1.5726	2	6 2 0	58.66	
1.5164	9	5 3 3	61.06	
1.4991	2	6 2 2	61.84	
1.3291	2	6 4 2	70.84	
1.2947	14	7 3 1+	73.02	
1.2431	9	8 0 0	76.58	
1.2149	1	7 3 3	78.70	
1.2059	1	6 4 4+	79.40	
1.1720	1	8 2 2+	82.18	
1.1483	7	7 5 1+	84.26	
1.1408	1	6 6 2	84.94	
1.0850	1	8 4 2	90.46	
1.0425	5	9 3 1	95.28	
1.0150	19	8 4 4	98.74	
.9751	1	8 6 2+	104.36	
.9614	6	9 5 1+	106.50	
.9570	1	10 2 2+	107.20	
.9233	1	10 4 0+	113.08	
.8967	3	11 1 1+	118.42	
.8790	7	8 8 0	122.40	
.8435	4	9 7 3+	131.90	
.8405	1	10 6 2	132.82	
.8067	1	10 6 4+	145.46	
.7988	6	9 7 5+	149.30	
.7862	14	12 4 0	156.90	

Cobalt ruthenium sulfide, Co₈RuS₈ - (continued)

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å
5.742	7	1 1 1	15.42	
4.973	10	2 0 0	17.82	
3.516	11	2 2 0	25.31	
2.999	100	3 1 1	29.77	
2.871	10	2 2 2	31.13	
2.486	3	4 0 0	36.10	
2.282	6	3 3 1	39.46	
2.224	7	4 2 0	40.53	
2.030	4	4 2 2	44.60	
1.9139	30	5 1 1	47.47	
1.9139	8	3 3 3	47.47	
1.7580	85	4 4 0	51.97	
1.6810	1	5 3 1	54.55	
1.6575	1	6 0 0	55.39	
1.6575	2	4 4 2	55.39	
1.5724	2	6 2 0	58.66	
1.5166	11	5 3 3	61.05	
1.4993	2	6 2 2	61.83	
1.4354	1	4 4 4	64.91	
1.3926	1	7 1 1	67.17	
1.3290	2	6 4 2	70.85	
1.2947	11	7 3 1	73.02	
1.2947	7	5 5 3	73.02	
1.2431	12	8 0 0	76.58	
1.2150	1	7 3 3	78.69	
1.2060	1	6 4 4	79.39	
1.1483	8	7 5 1	84.26	
1.1483	2	5 5 5	84.26	
1.1408	1	6 6 2	84.95	
1.0851	1	8 4 2	90.45	
1.0425	6	9 3 1	95.27	
1.0150	25	8 4 4	98.74	
.9752	1	8 6 2	104.35	
.9614	2	7 7 3	106.49	
.9614	6	9 5 1	106.49	
.9234	1	10 4 0	113.07	
.9079	1	10 4 2	116.10	
.8967	2	11 1 1	118.42	
.8967	2	7 7 5	118.42	
.8790	11	8 8 0	122.40	
.8689	1	11 3 1	124.88	
.8435	6	9 7 3	131.90	
.8435	2	11 3 3	131.90	
.8405	1	10 6 2	132.83	
.8066	2	10 6 4	145.47	
.7988	9	9 7 5	149.30	
.7988	7	11 5 3	149.30	
.7862	47	12 4 0	156.90	

Cobalt tantalum silicide, $\text{Co}_{16}\text{Ta}_6\text{Si}_7$

Structure

Cubic, $\text{Fm}\bar{3}\text{m}$ (225), $Z = 4$, isostructural with $\text{Cu}_{16}\text{Mg}_6\text{Si}_7$, from powder data [Spiegel et al., 1963]. Kuz'ma et al. [1964] determined positions for $\text{Co}_{16}\text{Nb}_6\text{Si}_7$, a similar isostructural compound.

Atom positions

From considerations of atomic size, the positions of $\text{Co}_{16}\text{Nb}_6\text{Si}_7$ were preferred.

32(f) 32 cobalt (1)
32(f) 32 cobalt (2)
4(b) 4 silicon (1)
24(d) 24 silicon (2)
24(e) 24 tantalum

Lattice constant

$a = 11.199 \text{ \AA}$
(published value, 11.198 \AA [Spiegel et al., 1963]).

Volume

1404.6 \AA^3

Density

(calculated) 10.523 g/cm^3

Thermal parameters

Isotropic: cobalt $B = 1.0$; silicon $B = 1.0$;
tantalum $B = 0.8$.

Scattering factors

Co^0 , Si^0 , Ta^0 [International Tables, 1962]

Scale factor (integrated intensities)

$\gamma = 0.361 \times 10^{-3}$

References

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.), pp. 202, 204, 212.
Kuz'ma, Yu. B., Gladyshevs'kii, E. I., and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.
Spiegel, F. X., Bardos, D., and Beck, P. A. (1963). Trans. AIME 227, 575.

Calculated Pattern (Peak heights)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598 \text{ \AA}$
6.458	25	1 1 1	13.70	
5.597	8	2 0 0	15.82	
3.959	1	2 2 0	22.44	
3.232	40	2 2 2	27.58	
2.800	2	4 0 0	31.94	
2.569	30	3 3 1	34.90	
2.504	6	4 2 0	35.84	
2.286	35	4 2 2	39.38	
2.155	100	5 1 1+	41.88	
1.980	45	4 4 0	45.80	
1.893	3	5 3 1	48.02	
1.866	25	6 0 0	48.76	
1.568	12	5 5 1	58.84	
1.553	4	6 4 0	59.48	
1.458	8	7 3 1+	63.78	
1.400	2	8 0 0	66.78	
1.368	9	7 3 3	68.52	
1.358	2	6 4 4+	69.10	
1.320	20	8 2 2+	71.42	
1.293	11	5 5 5+	73.12	
1.229	4	7 5 3	77.60	
1.222	9	8 4 2	78.16	
1.125	14	9 3 3+	86.38	
1.120	2	10 0 0	86.92	
1.098	3	10 2 0+	89.08	
1.083	6	7 7 3+	90.72	
1.078	3	6 6 6	91.26	
1.040	3	10 4 0	95.60	
1.010	2	11 1 1	99.44	
.9785	2	9 7 1+	103.86	
.9747	6	8 8 2+	104.42	
.9604	2	10 6 0	106.66	
.9499	1	9 7 3	108.38	
.9465	2	10 6 2	108.94	
.9332	4	8 8 4+	111.26	
.9236	4	11 5 1+	113.02	
.9083	5	10 6 4+	116.00	
.8995	1	11 5 3+	117.82	
.8854	2	12 4 0	120.92	
.8745	2	10 8 0+	123.50	
.8640	1	10 8 2	126.14	
.8564	8	11 5 5+	128.18	
.8542	5	10 6 6	128.78	
.8371	8	13 3 1+	133.92	
.8349	6	12 6 0	134.62	
.8256	1	12 6 2	137.82	
.8190	3	13 3 3+	140.30	

Cobalt tantalum silicide, Co₁₆Ta₆Si₇ - (Continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
6.466	40	1 1 1	13.68	
5.599	12	2 0 0	15.81	
3.959	2	2 2 0	22.44	
3.377	1	3 1 1	26.37	
3.233	70	2 2 2	27.57	
2.800	4	4 0 0	31.94	
2.569	50	3 3 1	34.89	
2.504	10	4 2 0	35.83	
2.286	60	4 2 2	39.38	
2.155	100	5 1 1	41.88	
2.155	85	3 3 3	41.88	
1.980	85	4 4 0	45.80	
1.893	6	5 3 1	48.02	
1.866	40	6 0 0	48.75	
1.866	6	4 4 2	48.75	
1.616	1	4 4 4	56.92	
1.568	25	5 5 1	58.84	
1.553	8	6 4 0	59.47	
1.458	11	7 3 1	63.79	
1.458	6	5 5 3	63.79	
1.400	5	8 0 0	66.77	
1.368	19	7 3 3	68.53	
1.358	3	6 4 4	69.11	
1.320	19	6 6 0	71.41	
1.320	25	8 2 2	71.41	
1.293	10	7 5 1	73.12	
1.293	13	5 5 5	73.12	
1.229	8	7 5 3	77.61	
1.222	18	8 4 2	78.16	
1.194	1	6 6 4	80.37	
1.143	1	8 4 4	84.74	
1.126	25	9 3 3	86.37	
1.126	2	7 7 1	86.37	
1.126	2	7 5 5	86.37	
1.120	3	10 0 0	86.92	
1.098	3	8 6 2	89.09	
1.098	3	10 2 0	89.09	
1.083	7	7 7 3	90.71	
1.083	6	9 5 1	90.71	
1.078	7	6 6 6	91.26	
1.040	6	10 4 0	95.60	
1.010	5	11 1 1	99.43	
.9899	1	8 8 0	102.19	
.9785	3	9 7 1	103.86	
.9785	1	9 5 5	103.86	
.9747	12	8 8 2	104.42	
.9747	2	10 4 4	104.42	
.9603	5	10 6 0	106.67	
.9499	2	9 7 3	108.38	
.9465	6	10 6 2	108.95	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
.9332	9	8 8 4	111.26	
.9332	2	12 0 0	111.26	
.9237	9	11 5 1	113.01	
.9237	2	7 7 7	113.01	
.9206	1	12 2 0	113.60	
.9084	4	12 2 2	115.99	
.9084	8	10 6 4	115.99	
.8995	2	11 5 3	117.82	
.8854	5	12 4 0	120.93	
.8745	2	12 4 2	123.49	
.8745	2	10 8 0	123.49	
.8745	2	8 8 6	123.49	
.8640	3	10 8 2	126.13	
.8564	15	11 5 5	128.17	
.8564	3	11 7 1	128.17	
.8564	5	9 9 3	128.17	
.8539	7	10 6 6	128.87	
.8371	16	13 3 1	133.93	
.8371	5	11 7 3	133.93	
.8371	6	9 7 7	133.93	
.8347	9	12 6 0	134.68	
.8256	4	12 6 2	137.82	
.8190	8	13 3 3	140.30	
.8190	5	9 9 5	140.30	
.8082	2	8 8 8	144.76	

Cobalt titanium silicide, $\text{Co}_{16}\text{Ti}_6\text{Si}_7$

Structure

Cubic, $\text{Fm}\bar{3}\text{m}$ (225), $Z = 4$, isostructural with $\text{Cu}_{16}\text{Mg}_6\text{Si}_7$, from powder data [Spiegel et al., 1963]. Kuz'ma et al. [1964] determined positions for $\text{Co}_{16}\text{Nb}_6\text{Si}_7$, a similar isostructural compound.

Atom positions

From considerations of atomic size, the positions for $\text{Co}_{16}\text{Nb}_6\text{Si}_7$ were preferred.

32(f)	32 cobalt (1)
32(f)	32 cobalt (2)
4(b)	4 silicon (1)
24(d)	24 silicon (2)
24(e)	24 titanium

Lattice constant

$a = 11.202 \text{ \AA}$
(published value, 11.201 \AA [Spiegel et al., 1963])

Volume

1405.7 \AA^3

Density

(calculated) 6.743 g/cm^3

Thermal parameters

Isotropic: overall $B = 1.0$

Scattering factors

Co^0 , Si^0 , Ti^0 [International Tables, 1962]

Scale factor (integrated intensities)

$\gamma = 0.215 \times 10^{-3}$

References

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 204.

Kuz'ma, Yu. B., Gladyshevs'kii, E. I., and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.
Spiegel, F. X., Bardos, D., and Beck, P. A. (1963). Trans. AIME 227, 575.

Calculated Pattern (Peak heights)

d (Å)	I	hkl	$2\theta (^\circ)$ $\lambda = 1.540598 \text{ \AA}$
6.458	6	1 1 1	13.70
5.597	30	2 0 0	15.82
3.959	3	2 2 0	22.44
3.234	2	2 2 2	27.56
2.800	20	4 0 0	31.94
2.570	4	3 3 1	34.88
2.505	7	4 2 0	35.82
2.286	20	4 2 2	39.38
2.155	90	5 1 1+	41.88
1.980	100	4 4 0	45.78
1.893	35	5 3 1	48.02
1.867	25	6 0 0	48.74
1.771	7	6 2 0	51.56
1.708	15	5 3 3	53.60
1.689	8	6 2 2	54.28
1.617	3	4 4 4	56.90
1.569	2	7 1 1+	58.82
1.497	1	6 4 2	61.94
1.459	2	7 3 1+	63.76
1.400	4	8 0 0	66.76
1.369	1	7 3 3	68.50
1.359	1	6 4 4+	69.08
1.320	14	6 6 0+	71.40
1.293	9	7 5 1+	73.10
1.230	11	7 5 3+	77.58
1.222	4	8 4 2	78.14
1.174	6	9 3 1	81.98
1.143	8	8 4 4	84.72
1.126	17	9 3 3	86.34
1.120	3	8 6 0	86.88
1.083	2	9 5 1+	90.68
1.078	5	6 6 6	91.22
1.040	1	10 4 0+	95.56
1.010	2	11 1 1+	99.40
.9901	4	8 8 0	102.16
.9787	6	9 7 1+	103.82
.9750	2	8 8 2	104.38
.9606	1	8 6 6	106.62
.9501	2	9 7 3+	108.34
.9468	4	10 6 2	108.90
.9335	3	8 8 4	111.22
.9208	1	12 2 0	113.56
.9086	1	10 6 4	115.94
.8856	3	12 4 0	120.88
.8567	5	11 5 5+	128.10
.8373	8	13 3 1+	133.86
.8351	7	12 6 0	134.56
.8258	2	12 6 2	137.74
.8192	2	9 9 5	140.22

Cobalt titanium silicide, $\text{Co}_{16}\text{Ti}_6\text{Si}_7$ - (Continued)

Calculated Pattern (Integrated)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
6.467	5	1 1 1	13.68	
5.601	25	2 0 0	15.81	
3.961	3	2 2 0	22.43	
3.234	2	2 2 2	27.56	
2.800	19	4 0 0	31.93	
2.570	4	3 3 1	34.88	
2.505	7	4 2 0	35.82	
2.287	19	4 2 2	39.37	
2.156	45	5 1 1	41.87	
2.156	40	3 3 3	41.87	
1.980	100	4 4 0	45.78	
1.893	35	5 3 1	48.01	
1.867	20	6 0 0	48.73	
1.867	3	4 4 2	48.73	
1.771	7	6 2 0	51.56	
1.708	15	5 3 3	53.61	
1.689	8	6 2 2	54.28	
1.617	4	4 4 4	56.90	
1.569	2	7 1 1	58.82	
1.497	1	6 4 2	61.94	
1.458	1	7 3 1	63.77	
1.458	1	5 5 3	63.77	
1.400	4	8 0 0	66.75	
1.369	2	7 3 3	68.51	
1.358	1	6 4 4	69.09	
1.320	10	6 6 0	71.39	
1.320	5	8 2 2	71.39	
1.293	6	7 5 1	73.10	
1.293	4	5 5 5	73.10	
1.252	1	8 4 0	75.91	
1.230	3	9 1 1	77.58	
1.230	9	7 5 3	77.58	
1.222	5	8 4 2	78.14	
1.194	1	6 6 4	80.34	
1.174	7	9 3 1	81.99	
1.143	9	8 4 4	84.71	
1.126	19	9 3 3	86.35	
1.126	1	7 7 1	86.35	
1.120	2	8 6 0	86.89	
1.098	1	10 2 0	89.06	
1.083	1	9 5 1	90.68	
1.078	5	6 6 6	91.22	
1.010	2	11 1 1	99.39	
.9901	5	8 8 0	102.15	
.9787	4	9 7 1	103.82	
.9787	3	11 3 1	103.82	
.9787	1	9 5 5	103.82	
.9750	2	8 8 2	104.38	
.9606	1	8 6 6	106.63	
.9501	1	9 7 3	108.33	

Calculated Pattern (Integrated)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
.9501	1	11 3 3	108.33	
.9467	5	10 6 2	108.90	
.9335	4	8 8 4	111.21	
.9208	1	12 2 0	113.56	
.9086	1	10 6 4	115.94	
.8856	4	12 4 0	120.87	
.8747	1	10 8 0	123.43	
.8643	1	10 8 2	126.07	
.8566	3	11 5 5	128.11	
.8566	1	11 7 1	128.11	
.8566	3	9 9 3	128.11	
.8373	7	13 3 1	133.85	
.8373	4	11 7 3	133.85	
.8373	3	9 7 7	133.85	
.8349	6	12 6 0	134.61	
.8258	4	12 6 2	137.74	
.8192	5	9 9 5	140.22	
.8084	1	8 8 8	144.66	

Diazepam, C₁₆H₁₃ClN₂O

Synonym

7-chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one

Structure

Monoclinic, P2₁/a (14), Z = 4. The structure was determined by Camerman and Camerman[1972].

Atom positions

All the atoms were in general positions. The value of 0.2274 was used for the x coordinate of carbon (5).

Lattice constants

a = 12.929(4) Å
b = 13.355(7)
c = 7.976(2)
β = 90.01(3)°
(published values: a=12.9284(41), b=13.3537(68)
c=7.9763(17), β=90.010(25)° [Camerman and Camerman, 1972]).

CD cell: a = 12.929, b = 13.355, c = 7.976,
β = 90.01, space group P2₁/a; a/b = 0.9681,
c/b = 0.5972

Volume

1377.2 Å³

Density

(measured) 1.39 g/cm³
(calculated) 1.37 g/cm³

Thermal parameters

Isotropic: overall B = 3.0

Scattering factors

C⁰, H⁰, N⁰, O⁰, Cl⁰ [International Tables, 1962]

Scale factors (integrated intensities)

γ = 0.575 × 10⁻³
I/I_c (calculated) = 0.64

Additional pattern

1. MacDonald et al. [1972]

References

Camerman, A. and Camerman, C. (1972). J. Amer. Chem. Soc. 94, 268.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

MacDonald, A., Michaelis, A. F., and Senkowski, B. Z. (1972). In Analytical Profiles of Drug Substances I (1972). (Academic Press, N. Y.), p. 79.

Calculated Pattern (Peak heights)

d(Å)	I	hkl	2θ(°) λ = 1.540598Å
9.28	33	1 1 0	9.52
7.96	22	0 0 1	11.10
6.84	2	0 1 1	12.94
6.67	9	0 2 0	13.26
6.46	31	2 0 0	13.70
6.05	6	-1 1 1	14.64
5.93	1	1 2 0	14.92
5.12	11	0 2 1	17.32
5.02	20	2 0 1	17.66
4.70	100	-2 1 1	18.88
4.64	77	2 2 0	19.10
4.21	3	1 3 0	21.10
4.10	5	3 1 0	21.66
4.01	16	-2 2 1+	22.14
3.887	84	0 3 1	22.86
3.821	5	0 1 2	23.26
3.720	41	1 3 1+	23.90
3.645	12	-3 1 1	24.40
3.619	21	3 2 0	24.58
3.394	6	2 0 2	26.24
3.331	16	-2 3 1+	26.74
3.309	9	1 2 2	26.92
3.297	11	-3 2 1+	27.02
3.232	12	1 4 0	27.58
3.140	4	4 1 0	28.40
3.079	2	0 4 1	28.98
3.026	14	-2 2 2+	29.50
2.996	23	1 4 1+	29.80
2.967	4	2 4 0	30.10
2.923	11	-4 1 1+	30.56
2.886	15	-3 3 1+	30.96
2.779	6	-2 4 1	32.18
2.733	1	4 2 1	32.74
2.698	5	2 3 2+	33.18
2.681	8	-3 2 2	33.40
2.639	3	3 4 0	33.94
2.556	1	0 4 2+	35.08
2.538	1	5 1 0	35.34
2.510	5	1 4 2+	35.74
2.506	5	-3 4 1+	35.80
2.485	2	1 5 1+	36.12
2.458	1	2 0 3+	36.52
2.418	6	-2 1 3+	37.16
2.413	7	5 2 0	37.24
2.379	3	2 4 2+	37.78
2.358	4	2 5 1+	38.14
2.352	4	-4 2 2+	38.24
2.308	2	2 2 3+	39.00
2.270	1	3 5 0	39.68
2.248	2	-1 3 3+	40.08

Diazepam, C₁₆H₁₃ClN₂O - (Continued)

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
2.230	3	-3 1 3 ⁺	40.42	
2.183	6	3 5 1 ⁺	41.32	
2.152	4	-5 3 1 ⁺	41.94	
2.144	3	3 2 3 ⁺	42.12	
2.127	2	6 1 0	42.46	
2.099	2	-2 5 2 ⁺	43.06	
2.080	2	0 4 3 ⁺	43.48	
2.063	4	-5 2 2 ⁺	43.84	
2.059	3	4 5 0 ⁺	43.94	
2.016	1	3 3 3 ⁺	44.92	
2.007	4	-4 4 2 ⁺	45.14	
1.986	2	6 2 1	45.64	
1.980	2	-5 4 1 ⁺	45.78	
1.972	5	0 1 4 ⁺	45.98	
1.950	2	5 3 2 ⁺	46.54	
1.922	1	1 6 2	47.26	
1.910	1	0 2 4	47.56	
1.895	1	-6 0 2	47.96	
1.885	4	0 5 3 ⁺	48.24	
1.873	2	3 4 3 ⁺	48.56	
1.865	2	-4 3 3 ⁺	48.80	
1.836	1	-5 1 3 ⁺	49.60	
1.830	2	2 7 0 ⁺	49.80	
1.819	1	5 4 2 ⁺	50.10	
1.809	3	2 5 3	50.40	
1.780	3	7 2 0 ⁺	51.28	
1.748	1	-2 3 4 ⁺	52.28	
1.721	1	0 7 2	53.18	
1.706	1	7 3 0 ⁺	53.68	
1.697	1	-4 0 4 ⁺	53.98	
1.684	1	-5 5 2 ⁺	54.44	
1.665	2	4 6 2 ⁺	55.10	
1.650	1	-2 6 3 ⁺	55.66	
1.621	1	-1 8 1 ⁺	56.74	
1.598	1	-3 7 2 ⁺	57.64	
1.584	1	2 8 1 ⁺	58.18	
1.549	1	-2 0 5 ⁺	59.66	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
9.29	34	1 1 0	9.51	
7.98	23	0 0 1	11.08	
6.85	2	0 1 1	12.92	
6.68	9	0 2 0	13.25	
6.46	37	2 0 0	13.69	
6.05	6	-1 1 1	14.63	
5.93	1	1 2 0	14.92	
5.12	12	0 2 1	17.31	
5.02	21	2 0 1	17.65	
4.76	1	-1 2 1	18.62	
4.76	2	1 2 1	18.63	
4.70	100	-2 1 1	18.86	
4.70	8	2 1 1	18.86	
4.64	79	2 2 0	19.09	
4.21	3	1 3 0	21.09	
4.10	5	3 1 0	21.65	
4.01	13	-2 2 1	22.13	
4.01	5	2 2 1	22.13	
3.887	100	0 3 1	22.86	
3.821	3	0 1 2	23.26	
3.723	15	-1 3 1	23.88	
3.722	32	1 3 1	23.89	
3.666	3	2 3 0	24.26	
3.664	1	1 1 2	24.27	
3.648	9	-3 1 1	24.38	
3.621	23	3 2 0	24.56	
3.394	7	2 0 2	26.24	
3.331	10	-2 3 1	26.74	
3.331	8	2 3 1	26.74	
3.310	5	1 2 2	26.92	
3.297	5	-3 2 1	27.02	
3.297	2	3 2 1	27.02	
3.290	3	-2 1 2	27.08	
3.289	1	2 1 2	27.09	
3.233	13	1 4 0	27.57	
3.142	4	4 1 0	28.39	
3.096	1	3 3 0	28.81	
3.080	2	0 4 1	28.97	
3.026	11	-2 2 2	29.50	
3.025	6	2 2 2	29.50	
2.996	7	-1 4 1	29.80	
2.996	12	1 4 1	29.80	
2.995	8	4 0 1	29.80	
2.966	3	2 4 0	30.10	
2.923	7	-4 1 1	30.56	
2.923	6	4 1 1	30.56	
2.895	6	-1 3 2	30.86	
2.887	8	-3 3 1	30.95	
2.886	8	3 3 1	30.96	
2.780	7	-2 4 1	32.17	

Diazepam, C₁₆H₁₃ClN₂O - (Continued)

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å
2.780	1	2 4 1	32.17	
2.733	1	4 2 1	32.74	
2.699	2	-2 3 2	33.16	
2.699	3	2 3 2	33.17	
2.681	9	-3 2 2	33.39	
2.639	3	3 4 0	33.94	
2.539	1	5 1 0	35.33	
2.511	4	1 4 2	35.73	
2.511	1	4 0 2	35.73	
2.506	1	-3 4 1	35.81	
2.506	1	3 4 1	35.81	
2.485	2	1 5 1	36.11	
2.459	1	2 0 3	36.52	
2.419	3	5 1 1	37.14	
2.418	4	-2 1 3	37.15	
2.418	1	2 1 3	37.15	
2.411	4	5 2 0	37.26	
2.380	1	-2 4 2	37.76	
2.380	2	2 4 2	37.77	
2.358	2	-2 5 1	38.13	
2.358	4	2 5 1	38.13	
2.351	2	-4 2 2	38.26	
2.307	1	2 2 3	39.01	
2.270	2	3 5 0	39.67	
2.248	1	-1 3 3	40.08	
2.231	2	-3 1 3	40.39	
2.230	1	-4 4 1	40.42	
2.230	1	4 4 1	40.42	
2.194	2	1 6 0	41.12	
2.187	1	-1 5 2	41.24	
2.187	1	4 3 2	41.25	
2.184	1	-3 5 1	41.31	
2.184	6	3 5 1	41.31	
2.153	3	-5 3 1	41.93	
2.153	1	5 3 1	41.93	
2.152	1	2 3 3	41.94	
2.143	1	-3 2 3	42.13	
2.143	2	3 2 3	42.13	
2.127	3	6 1 0	42.46	
2.099	2	-2 5 2	43.06	
2.099	1	2 5 2	43.06	
2.080	1	0 4 3	43.48	
2.064	3	-5 2 2	43.84	
2.063	1	5 2 2	43.84	
2.059	1	4 5 0	43.94	
2.055	1	6 1 1	44.02	
2.007	4	-4 4 2	45.14	
2.007	1	4 4 2	45.15	
1.986	2	6 2 1	45.64	
1.973	2	-3 5 2	45.96	

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å
1.973	2	3 5 2	45.96	
1.972	3	0 1 4	45.98	
1.950	1	5 3 2	46.53	
1.950	1	1 1 4	46.55	
1.922	2	1 6 2	47.25	
1.911	1	0 2 4	47.55	
1.896	1	-6 0 2	47.94	
1.890	1	-1 2 4	48.10	
1.885	2	-6 3 1	48.25	
1.884	2	0 5 3	48.26	
1.873	2	3 4 3	48.57	
1.865	1	-4 3 3	48.80	
1.836	1	-5 1 3	49.61	
1.830	1	2 7 0	49.79	
1.829	1	4 5 2	49.80	
1.819	1	5 4 2	50.10	
1.809	3	2 5 3	50.41	
1.787	1	-4 6 1	51.08	
1.780	3	7 2 0	51.28	
1.721	1	0 7 2	53.18	
1.706	1	7 3 0	53.68	
1.684	1	-5 5 2	54.44	
1.666	1	4 6 2	55.09	
1.650	1	-2 6 3	55.65	
1.621	1	-1 8 1	56.74	
1.584	1	2 8 1	58.19	
1.549	1	-2 0 5	59.65	

(N,N)-Dimethyltryptamine, C₁₂H₁₆N₂

Synonyms

DMT, 3-[2-(dimethylamino)-ethyl]indole

Structure

Monoclinic, P₂₁/c (14), Z = 8. The structure was determined by Falkenberg [1972].

Atom positions [ibid.]

All the atoms were in general positions, with 2 molecules in the asymmetric unit.

Polymorphism [ibid.]

The batch of the material described here also contained crystals of an entirely different polymorph. The latter could easily be distinguished by its optical properties and crystal shape, and had the monoclinic space group P₂₁/c with Z = 4.

Lattice constants [ibid.]

a = 12.99(1) Å
b = 12.08(1)
c = 18.38(2)
β = 127.85(1)°

CD cell: a = 14.61, b = 12.08, c = 12.99,
β = 96.73°, space group P₂₁/n; a/b = 1.2098,
c/b = 1.0753

Volume

2278. Å³

Density

(measured) 1.080 g/cm³
(calculated) 1.098 g/cm³

Thermal parameters

Isotropic: overall B = 5.0

Scattering factors

C⁰, H⁰, N⁰ [International Tables, 1962]

Scale factors (integrated intensities)

γ = 1.321 × 10⁻³
I/I_c (calculated) = 0.39

Additional pattern

1. Folen [1975].

References

Falkenberg, G. (1972). Acta Crystallogr. B28, 3075.
Folen, V. A. (1975). J. Forens. Sci. 20, 348.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkl	2θ(°)
λ = 1.540598Å			
9.28	47	0 1 1	9.52
8.80	14	-1 1 1	10.04
7.81	4	1 1 0	11.32
7.27	15	-1 1 2+	12.16
6.45	45	-2 0 2	13.72
6.21	100	0 1 2	14.24
6.04	49	0 2 0	14.66
5.68	7	-2 1 2	15.58
5.57	11	0 2 1	15.90
5.49	51	-2 1 1	16.14
5.40	7	-1 1 3	16.40
5.20	14	1 2 0	17.04
5.12	22	2 0 0+	17.30
5.04	8	-1 2 2	17.60
4.71	35	1 0 2	18.82
4.64	48	0 2 2	19.12
4.56	7	-2 0 4	19.46
4.48	68	1 2 1+	19.80
4.41	17	-2 2 2	20.14
4.36	31	-1 0 4	20.34
4.31	61	-2 2 1	20.58
4.26	99	-2 1 4+	20.82
4.13	73	-2 2 3	21.52
4.05	6	-3 1 3	21.92
4.00	22	-3 0 4	22.22
3.89	12	2 1 1	22.86
3.79	35	-3 1 4	23.44
3.71	12	1 2 2+	23.94
3.64	16	-2 2 4	24.44
3.53	11	-1 2 4	25.18
3.51	23	-2 1 5+	25.36
3.45	3	1 3 1	25.84
3.42	7	3 0 0	26.06
3.37	14	-2 3 1+	26.40
3.33	10	-3 2 4	26.72
3.28	12	-3 2 1+	27.18
3.22	11	-4 0 4+	27.72
3.17	2	2 3 0	28.16
3.11	14	-4 1 4	28.64
3.10	8	1 2 3+	28.82
3.06	3	1 3 2	29.14
3.02	6	-2 0 6+	29.60
2.976	3	-4 1 5+	30.00
2.951	5	-3 1 6+	30.26
2.919	2	2 2 2	30.60
2.864	6	3 1 1	31.20
2.845	3	-4 2 4+	31.42
2.826	3	-4 0 6+	31.64
2.746	4	-4 2 2+	32.58
2.712	10	-2 3 5+	33.00

(N,N)-Dimethyltryptamine, C₁₂H₁₆N₂ - (Continued)

Calculated Pattern (Peak heights)					
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å	
2.651	2	-3 3 5+	33.78		
2.618	4	1 2 4	34.22		
2.606	5	3 3 0+	34.38		
2.560	6	-4 2 6+	35.02		
2.483	1	-2 1 7	36.14		
2.464	3	-3 4 2	36.44		
2.448	3	-4 3 2	36.68		
2.443	3	-4 3 5	36.76		
2.413	3	-2 3 6	37.24		
2.382	2	1 1 5+	37.74		
2.360	2	4 2 0	38.10		
2.348	2	3 2 2	38.30		
2.303	5	-5 1 7	39.08		
2.262	1	-2 5 2	39.82		
2.255	1	-1 4 5+	39.94		
2.241	3	-4 1 8+	40.20		
2.239	3	2 4 2	40.24		
2.221	1	-2 5 3	40.58		
2.200	2	-3 3 7+	41.00		
2.186	2	2 5 0+	41.26		
2.173	1	-1 2 7+	41.52		
2.153	2	-4 4 2+	41.92		
2.139	2	-5 1 8+	42.22		
2.134	2	-6 0 4+	42.32		
2.114	1	-6 1 6+	42.74		
2.098	1	-6 1 4+	43.08		
2.063	1	-4 4 6+	43.84		
2.055	1	1 1 6+	44.02		
2.039	1	-1 4 6+	44.40		
2.027	2	-5 3 7+	44.68		
2.007	2	1 5 3+	45.14		
1.984	2	-4 3 8+	45.70		
1.967	1	-1 5 5+	46.10		
1.959	2	3 0 4	46.30		
1.943	1	5 2 0+	46.72		
1.934	1	-4 2 9+	46.94		
1.922	1	-2 6 2+	47.26		
1.897	2	-2 6 3+	47.92		
1.874	2	2 6 0+	48.54		
1.856	2	-6 3 7+	49.04		
1.852	2	1 6 2	49.16		
1.843	1	0 3 7+	49.40		
1.824	1	-5 0 10+	49.96		
1.798	2	-3 3 9+	50.72		
1.783	1	2 1 6+	51.20		
1.761	1	-7 2 7+	51.88		
1.727	1	-7 2 8+	52.98		
1.678	1	0 7 2+	54.66		
1.670	1	-4 3 10+	54.94		
1.659	1	-7 0 10+	55.34		
1.642	1	-4 1 11+	55.94		

Calculated Pattern (Integrated)					
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å	
9.28	46	0 1 1	9.52		
9.13	2	-1 0 2	9.68		
8.82	14	-1 1 1	10.02		
7.82	4	1 1 0	11.31		
7.28	11	-1 1 2	12.15		
7.26	5	0 0 2	12.19		
6.45	45	-2 0 2	13.72		
6.22	100	0 1 2	14.23		
6.04	47	0 2 0	14.65		
5.69	6	-2 1 2	15.56		
5.58	7	0 2 1	15.88		
5.49	49	-2 1 1	16.12		
5.47	7	-1 2 1	16.19		
5.40	4	-1 1 3	16.42		
5.20	12	1 2 0	17.02		
5.13	18	2 0 0	17.28		
5.12	5	-2 1 3	17.30		
5.04	7	-1 2 2	17.59		
4.72	3	2 1 0	18.78		
4.71	31	1 0 2	18.81		
4.64	48	0 2 2	19.10		
4.56	2	-2 0 4	19.44		
4.49	40	0 1 3	19.75		
4.48	43	1 2 1	19.82		
4.41	10	-2 2 2	20.12		
4.36	25	-1 0 4	20.33		
4.32	55	-2 2 1	20.56		
4.27	66	-2 1 4	20.79		
4.27	22	-1 2 3	20.80		
4.26	19	-3 0 2	20.83		
4.13	77	-2 2 3	21.51		
4.10	6	-1 1 4	21.63		
4.05	3	-3 1 3	21.92		
4.02	2	-3 1 2	22.10		
4.00	22	-3 0 4	22.22		
3.89	11	2 1 1	22.85		
3.80	38	-3 1 4	23.42		
3.78	2	0 2 3	23.54		
3.72	8	1 2 2	23.92		
3.72	4	-3 1 1	23.93		
3.64	17	-2 2 4	24.43		
3.63	1	0 0 4	24.51		
3.54	9	-1 2 4	25.15		
3.51	20	-2 1 5	25.35		
3.50	7	-3 2 3	25.41		
3.47	1	0 1 4	25.61		
3.45	2	1 3 1	25.83		
3.42	6	3 0 0	26.04		
3.40	5	2 2 1	26.21		
3.38	6	-3 1 5	26.33		

(N,N)-Dimethyltryptamine, C₁₂H₁₆N₂ - (Continued)

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å
3.37	11	-2 3 1	26.41	
3.35	2	-1 3 3	26.60	
3.33	10	-3 2 4	26.72	
3.29	2	3 1 0	27.08	
3.28	1	-2 3 3	27.17	
3.28	10	-3 2 1	27.17	
3.23	9	-4 0 4	27.64	
3.21	7	2 1 2	27.74	
3.17	1	2 3 0	28.15	
3.12	14	-4 1 4	28.62	
3.11	1	0 2 4	28.68	
3.10	5	1 2 3	28.82	
3.09	1	0 3 3	28.82	
3.08	2	-4 0 2	28.92	
3.06	3	1 3 2	29.14	
3.02	2	0 4 0	29.55	
3.02	3	-2 3 4	29.56	
3.02	3	-2 0 6	29.61	
2.978	2	-4 1 5	29.98	
2.975	1	3 2 0	30.01	
2.960	1	-1 3 4	30.17	
2.957	2	-1 2 5	30.20	
2.950	3	-3 1 6	30.27	
2.939	2	-3 3 3	30.39	
2.919	1	2 2 2	30.61	
2.906	1	1 0 4	30.75	
2.876	3	2 3 1	31.08	
2.864	5	3 1 1	31.20	
2.848	1	-4 2 3	31.39	
2.845	2	-4 2 4	31.42	
2.827	3	-4 0 6	31.63	
2.822	1	0 1 5	31.68	
2.752	1	-4 1 6	32.50	
2.747	3	-4 2 2	32.57	
2.735	1	-2 4 2	32.72	
2.717	1	-3 2 6	32.94	
2.712	2	-2 4 1	33.00	
2.712	8	-2 3 5	33.00	
2.698	3	-2 2 6	33.18	
2.695	1	0 3 4	33.21	
2.651	2	-3 3 5	33.78	
2.618	4	1 2 4	34.22	
2.606	4	3 3 0	34.38	
2.602	1	2 4 0	34.44	
2.566	4	-3 1 7	34.94	
2.560	4	-4 2 6	35.02	
2.543	1	1 4 2	35.26	
2.484	1	-2 1 7	36.13	
2.471	1	-3 4 3	36.32	
2.464	3	-3 4 2	36.44	

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å
2.449	2	-4 3 2	36.67	
2.443	1	-4 3 5	36.76	
2.413	4	-2 3 6	37.23	
2.382	1	1 1 5	37.74	
2.360	2	4 2 0	38.09	
2.348	1	3 2 2	38.31	
2.303	5	-5 1 7	39.08	
2.262	1	-2 5 2	39.81	
2.243	1	-1 5 3	40.18	
2.242	1	-4 1 8	40.19	
2.238	2	2 4 2	40.26	
2.222	1	-2 5 3	40.57	
2.204	1	-4 4 4	40.91	
2.199	2	-3 3 7	41.00	
2.158	1	-4 4 2	41.83	
2.139	1	-5 1 8	42.22	
2.134	1	-4 2 8	42.31	
2.131	1	-6 0 4	42.39	
2.098	1	-6 1 4	43.08	
2.039	1	-1 4 6	44.40	
2.027	1	-5 3 7	44.67	
2.007	1	1 5 3	45.14	
1.985	1	-4 3 8	45.67	
1.983	1	-1 1 8	45.71	
1.960	2	3 0 4	46.30	
1.934	1	-4 2 9	46.94	
1.898	1	-6 2 8	47.90	
1.897	2	-2 6 3	47.92	
1.874	1	2 6 0	48.54	
1.856	1	-6 3 7	49.04	
1.852	1	1 6 2	49.17	
1.799	1	-6 2 9	50.70	
1.798	1	-3 3 9	50.72	
1.783	1	2 1 6	51.21	
1.763	1	-7 2 7	51.82	
1.727	1	-7 2 8	52.98	
1.679	1	0 7 2	54.62	
1.670	1	-7 2 9	54.92	
1.670	1	-4 3 10	54.95	

Methapyrilene hydrochloride, $C_{14}H_{20}ClN_3S$

Synonyms

1. 2-[(2)-dimethylaminoethyl-2-thenylamino]-pyridine hydrochloride
2. thenylpyramine hydrochloride

Structure

Monoclinic, $P2_1/c$ (14), $Z = 8$. The structure was determined by Clark and Palenik [1972]. There were two molecules in the asymmetric unit and in one of them the thiophene ring was disordered; one sulfur and one carbon atom shared occupancy of each of 2 sites, on an approximately equal basis.

Atom positions

Three hydrogen atoms on the disordered thiophene ring were omitted from the refinement and their positions not determined. All other atoms were in general positions.

Lattice constants.

$a = 10.937(3)$ Å
 $b = 10.418(3)$
 $c = 28.258(8)$
 $\beta = 106.21(2)^\circ$
 (published values: $a = 10.936$, $b = 10.417$
 $c = 28.256$, $\beta = 106.21^\circ$ [Clark and Palenik, 1972])
 CD cell: $a = 27.305$, $b = 10.418$, $c = 10.937$,
 $\beta = 96.41^\circ$, space group $P2_1/n$, $a/b = 2.6209$,
 $c/b = 1.0498$

Volume

3091.8 \AA^3

Density

(measured) 1.273 g/cm^3
 (calculated) 1.280 g/cm^3

Thermal parameters

Isotropic: overall $B = 5.0$

Scattering factors

C^0 , H^0 , Cl^0 , N^0 , S^0 [International Tables, 1962]

Scale factors (integrated intensities)

$\gamma = 0.213 \times 10^{-3}$
 I/I_c (calculated) = 0.35

Additional pattern

1. PDF 12-872 [Rose and Williams, 1959]

References

Clark, G. R. and Palenik, G. J. (1972). J. Amer. Chem. Soc. 94, 4005.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
 Rose, H. A. and Williams, J. G. (1959). J. Amer. Pharm. Ass. 48, 487.

Calculated Pattern (Peak heights)

$d(\text{\AA})$	I	hkl	$2\theta(^\circ)$ $\lambda = 1.540598\text{\AA}$
9.71	3	0 1 1	9.10
8.26	7	0 1 2	10.70
7.52	60	-1 1 1	11.76
7.10	10	-1 1 2	12.46
6.79	26	1 1 1*	13.02
6.59	3	-1 0 4	13.42
6.37	5	-1 1 3	13.90
6.01	1	1 1 2	14.72
5.68	13	0 1 4	15.58
5.58	2	-1 1 4	15.88
5.43	5	-2 0 2	16.30
5.21	40	0 2 0	17.02
4.85	93	-2 0 4*	18.26
4.69	20	2 1 0	18.92
4.59	8	-1 2 2	19.34
4.52	47	0 0 6	19.62
4.37	24	-1 2 3	20.30
4.25	7	-1 1 6	20.90
4.13	100	2 1 2*	21.52
4.02	37	-2 0 6*	22.10
3.757	67	-2 1 6*	23.66
3.684	53	2 0 4*	24.14
3.553	38	-2 2 4	25.04
3.469	10	-1 2 6	25.66
3.437	5	-2 1 7*	25.90
3.401	15	-3 1 1*	26.18
3.341	7	1 2 5*	26.66
3.300	4	-2 0 8*	27.00
3.269	2	-1 3 2	27.26
3.225	4	0 1 8	27.64
3.186	17	1 1 7*	27.98
3.144	23	-2 1 8	28.36
3.091	2	0 3 4	28.86
3.064	2	1 2 6*	29.12
3.008	20	2 2 4*	29.68
2.974	16	-3 2 3*	30.02
2.912	21	2 1 6	30.68
2.879	6	3 1 3*	31.04
2.850	2	-3 2 5	31.36
2.834	3	2 3 1	31.54
2.788	5	-2 2 8	32.08
2.746	3	0 3 6*	32.58
2.736	3	-2 3 5	32.70
2.715	9	-4 0 4*	32.96
2.688	2	-1 2 9	33.30
2.679	2	2 1 7	33.42
2.651	2	-2 1 10	33.78
2.626	6	-1 3 7*	34.12
2.623	6	1 1 9*	34.16
2.601	7	-2 2 9*	34.46

Methapyrilene hydrochloride, $C_{14}H_{20}ClN_3S$ - (Continued)

Calculated Pattern (Peak heights)					
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å	
2.546	9	3 1 5*	35.22		
2.527	6	2 3 4*	35.50		
2.502	6	1 4 1*	35.86		
2.475	7	-1 4 3*	36.26		
2.449	3	4 0 2*	36.66		
2.430	7	0 4 4*	36.96		
2.409	3	1 3 7*	37.30		
2.391	4	1 4 3*	37.58		
2.388	4	-3 2 9*	37.64		
2.367	2	-4 1 8	37.98		
2.346	4	3 2 5*	38.34		
2.332	4	-4 2 6*	38.58		
2.301	1	-1 2 11*	39.12		
2.285	2	2 3 6*	39.40		
2.276	2	0 3 9	39.56		
2.272	2	-1 4 6*	39.64		
2.262	1	0 0 12*	39.82		
2.246	1	3 1 7*	40.12		
2.222	3	-4 0 10*	40.56		
2.213	3	1 1 11*	40.74		
2.194	1	2 4 3*	41.10		
2.175	3	2 0 10	41.48		
2.152	2	-2 3 10	41.94		
2.138	4	-4 3 2*	42.24		
2.133	4	1 3 9	42.34		
2.128	4	2 1 10*	42.44		
2.124	4	-2 2 12*	42.52		
2.094	1	3 3 5*	43.16		
2.069	2	-3 4 5	43.72		
2.063	3	4 2 4*	43.86		
2.044	2	1 5 0*	44.28		
2.038	2	-1 5 2*	44.42		
2.030	3	0 5 3*	44.60		
2.010	2	-2 0 14*	45.08		
1.999	5	4 1 6	45.32		
1.982	1	-3 4 7	45.74		
1.973	3	-2 1 14*	45.96		
1.947	2	4 3 3*	46.62		
1.939	3	0 0 14*	46.82		
1.933	2	-2 3 12*	46.96		
1.929	2	-3 4 8	47.08		
1.917	2	3 3 7*	47.38		
1.890	3	2 5 2	48.10		
1.872	2	-5 2 9*	48.60		
1.863	2	2 1 12	48.84		
1.858	2	-3 3 12	48.98		
1.850	1	4 4 0*	49.22		
1.843	2	-1 1 15*	49.42		
1.822	3	-5 3 1*	50.02		
1.801	2	-3 1 15*	50.64		

Calculated Pattern (Peak heights)					
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å	
1.795	3	-4 1 14*	50.84		
1.791	2	1 4 10*	50.96		
1.775	3	-3 3 13*	51.44		
1.770	3	-6 0 8*	51.60		
1.750	1	6 0 0*	52.22		
1.744	2	-3 4 11*	52.42		
1.740	2	4 2 8*	52.56		
1.720	1	3 4 7*	53.22		
1.710	2	-6 2 6*	53.54		
1.697	1	-1 6 3*	54.00		
1.694	1	-3 3 14*	54.10		
1.668	2	4 0 10*	55.00		
1.659	1	-2 5 10*	55.34		
1.655	2	-1 6 5*	55.48		
1.619	1	-6 2 10*	56.84		
1.612	1	2 5 8*	57.08		
1.588	2	4 5 2*	58.02		
1.559	1	1 4 13*	59.22		
1.555	1	-4 1 17*	59.38		
1.550	1	-4 3 15*	59.58		
1.547	1	-7 1 5*	59.74		

Calculated Pattern (Integrated)					
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å	
9.73	3	0 1 1	9.09		
8.26	8	0 1 2	10.70		
7.52	72	-1 1 1	11.76		
7.40	5	1 1 0	11.96		
7.11	11	-1 1 2	12.44		
6.83	1	0 1 3	12.95		
6.80	20	1 1 1	13.00		
6.78	13	0 0 4	13.04		
6.60	2	-1 0 4	13.41		
6.37	6	-1 1 3	13.89		
6.02	1	1 1 2	14.71		
5.68	15	0 1 4	15.58		
5.58	2	-1 1 4	15.88		
5.43	6	-2 0 2	16.30		
5.25	18	2 0 0	16.87		
5.21	46	0 2 0	17.01		
4.86	11	0 2 2	18.23		
4.86	57	-2 0 4	18.24		
4.85	53	-1 1 5	18.26		
4.83	1	-2 1 1	18.37		
4.82	5	-2 1 2	18.40		
4.81	2	0 1 5	18.42		
4.69	21	2 1 0	18.91		
4.67	1	1 2 0	19.00		
4.67	6	-2 1 3	19.01		

Methapyrilene hydrochloride, C₁₄H₂₀ClN₃S -(Continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
4.59	6	-1 2 2	19.32	
4.52	58	0 0 6	19.61	
4.51	1	1 2 1	19.68	
4.49	4	2 0 2	19.74	
4.40	2	-2 1 4	20.14	
4.37	29	-1 2 3	20.29	
4.25	5	-1 1 6	20.90	
4.15	90	0 1 6	21.40	
4.13	1	0 2 4	21.49	
4.13	100	2 1 2	21.52	
4.09	2	-1 2 4	21.72	
4.09	18	-2 1 5	21.72	
4.03	33	-2 0 6	22.05	
4.02	21	1 1 5	22.12	
3.787	1	1 0 6	23.47	
3.765	2	-2 2 1	23.61	
3.760	42	-2 2 2	23.64	
3.757	46	-2 1 6	23.67	
3.750	3	-1 1 7	23.71	
3.698	22	2 2 0	24.04	
3.686	7	-2 2 3	24.12	
3.684	52	2 0 4	24.14	
3.640	1	1 2 4	24.44	
3.571	2	2 2 1	24.91	
3.559	1	1 1 6	25.00	
3.554	50	-2 2 4	25.04	
3.529	1	-1 0 8	25.22	
3.470	12	-1 2 6	25.65	
3.440	2	-3 1 2	25.88	
3.438	2	-2 1 7	25.89	
3.415	1	0 2 6	26.07	
3.404	11	-3 1 1	26.16	
3.402	7	2 2 2	26.17	
3.392	1	0 0 8	26.25	
3.364	3	0 3 2	26.47	
3.351	2	-3 1 4	26.58	
3.342	3	-1 1 8	26.65	
3.339	4	1 2 5	26.67	
3.300	4	-2 0 8	27.00	
3.270	1	-1 3 2	27.25	
3.242	1	0 3 3	27.49	
3.239	1	1 3 1	27.51	
3.225	3	0 1 8	27.64	
3.194	11	3 1 1	27.91	
3.186	2	-2 2 6	27.98	
3.186	13	1 1 7	27.99	
3.146	31	-2 1 8	28.35	
3.091	1	0 3 4	28.86	
3.073	1	-1 3 4	29.03	
3.063	1	1 2 6	29.13	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2θ(°)	λ = 1.540598Å
3.034	2	2 0 6	29.42	
3.014	8	1 3 3	29.62	
3.008	11	2 2 4	29.68	
3.006	9	-1 1 9	29.69	
2.985	12	-2 2 7	29.91	
2.974	13	-3 2 3	30.02	
2.963	9	-3 2 1	30.14	
2.933	7	-3 1 7	30.45	
2.926	2	-2 3 2	30.52	
2.925	3	0 3 5	30.54	
2.921	1	-1 2 8	30.58	
2.913	26	2 1 6	30.67	
2.884	1	-2 1 9	30.98	
2.879	5	3 1 3	31.04	
2.851	2	-3 2 5	31.35	
2.834	4	2 3 1	31.54	
2.788	7	-2 2 8	32.08	
2.754	2	0 3 6	32.48	
2.748	1	2 3 2	32.56	
2.743	1	-2 0 10	32.62	
2.736	1	-2 3 5	32.70	
2.723	4	-4 0 2	32.86	
2.717	7	-4 0 4	32.94	
2.714	2	1 3 5	32.97	
2.713	2	0 0 10	32.98	
2.689	1	-1 2 9	33.29	
2.678	1	2 1 7	33.44	
2.653	2	-2 1 10	33.76	
2.630	1	-2 3 6	34.06	
2.629	2	-4 1 4	34.07	
2.628	3	-1 3 7	34.09	
2.626	2	4 0 0	34.12	
2.621	1	2 2 6	34.18	
2.618	3	1 1 9	34.23	
2.609	1	0 2 9	34.34	
2.601	5	-2 2 9	34.46	
2.600	3	-3 1 9	34.47	
2.593	2	0 4 1	34.57	
2.558	2	0 4 2	35.05	
2.547	6	3 1 5	35.21	
2.546	5	4 1 0	35.22	
2.544	1	2 0 8	35.25	
2.533	1	-1 4 1	35.41	
2.528	2	1 4 0	35.48	
2.527	5	2 3 4	35.49	
2.516	1	-1 4 2	35.66	
2.507	2	-3 3 3	35.79	
2.502	6	1 4 1	35.87	
2.492	1	-1 1 11	36.02	
2.478	5	-1 4 3	36.22	

Methapyrilene hydrochloride, $C_{14}H_{20}ClN_3S$ - (Continued)

Calculated Pattern (Integrated)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
2.475	4	-1 3 8	36.27	
2.471	1	2 1 8	36.32	
2.453	2	4 0 2	36.60	
2.449	1	-2 1 11	36.66	
2.431	5	0 4 4	36.94	
2.430	3	-4 0 8	36.96	
2.426	2	0 3 8	37.02	
2.409	2	1 3 7	37.29	
2.393	3	1 4 3	37.55	
2.392	1	-2 3 8	37.57	
2.388	1	4 1 2	37.64	
2.387	2	-3 2 9	37.66	
2.367	2	-4 1 8	37.99	
2.345	3	3 2 5	38.35	
2.333	3	-4 2 6	38.57	
2.330	2	-2 4 3	38.61	
2.326	2	-2 0 12	38.68	
2.285	1	2 3 6	39.41	
2.277	2	0 3 9	39.55	
2.244	1	3 1 7	40.14	
2.222	3	-4 0 10	40.56	
2.213	2	1 1 11	40.74	
2.212	1	-3 3 8	40.76	
2.210	1	0 1 12	40.80	
2.194	1	2 4 3	41.10	
2.176	3	2 0 10	41.47	
2.153	3	-2 3 10	41.94	
2.143	1	4 2 3	42.12	
2.143	2	-4 3 2	42.13	
2.138	2	-5 1 3	42.23	
2.134	1	1 3 9	42.32	
2.130	2	2 1 10	42.41	
2.128	2	-5 1 5	42.45	
2.125	1	-4 3 1	42.51	
2.124	2	-2 2 12	42.53	
2.121	1	-1 1 13	42.60	
2.115	1	-3 4 3	42.72	
2.069	1	-3 4 5	43.71	
2.063	3	4 2 4	43.85	
2.059	2	0 5 2	43.93	
2.037	1	-1 5 2	44.43	
2.030	2	0 5 3	44.59	
2.030	1	-3 4 6	44.60	
2.030	1	1 5 1	44.61	
2.012	1	5 1 1	45.02	
2.010	1	-2 0 14	45.08	
1.999	6	4 1 6	45.32	
1.983	1	-3 4 7	45.73	
1.977	1	-4 1 12	45.86	
1.973	3	-2 1 14	45.96	

Calculated Pattern (Integrated)				
$d(\text{\AA})$	I	hkl	$2\theta(^{\circ})$	$\lambda = 1.540598\text{\AA}$
1.947	1	4 3 3	46.60	
1.941	1	-3 0 14	46.77	
1.938	2	0 0 14	46.84	
1.933	1	-2 3 12	46.98	
1.928	1	-3 4 8	47.09	
1.919	1	-3 2 13	47.33	
1.917	2	3 3 7	47.39	
1.902	1	-1 5 6	47.79	
1.890	3	2 5 2	48.10	
1.886	1	4 3 4	48.21	
1.882	1	-4 4 2	48.31	
1.878	1	-4 2 12	48.42	
1.872	1	-5 2 9	48.60	
1.863	2	2 1 12	48.84	
1.858	2	-3 3 12	48.98	
1.844	1	2 3 10	49.39	
1.843	1	-1 1 15	49.42	
1.842	1	4 0 8	49.44	
1.822	2	-5 3 1	50.01	
1.801	1	-3 1 15	50.64	
1.796	1	-3 5 4	50.81	
1.794	1	-1 5 8	50.85	
1.794	1	-4 1 14	50.86	
1.791	1	1 4 10	50.96	
1.780	1	2 2 12	51.29	
1.777	1	-4 4 8	51.38	
1.775	2	0 5 8	51.43	
1.774	2	-3 3 13	51.46	
1.770	2	-6 0 8	51.60	
1.750	1	6 0 0	52.22	
1.744	1	-3 4 11	52.42	
1.740	1	-2 1 16	52.57	
1.737	1	4 2 8	52.66	
1.723	1	3 4 7	53.10	
1.711	1	-6 2 6	53.52	
1.709	1	-4 1 15	53.58	
1.694	1	-3 3 14	54.09	
1.671	1	-2 2 16	54.90	
1.668	1	4 0 10	54.99	
1.665	1	2 5 7	55.10	
1.659	1	-2 5 10	55.32	
1.655	1	-1 6 5	55.46	
1.653	1	0 5 10	55.56	
1.588	1	4 5 2	58.03	
1.550	1	-4 3 15	59.58	

Silicon nitride, β -Si₃N₄

Structure

Hexagonal, P6₃/m (176), Z = 4. The structure was determined by Hardie and Jack [1957].

Atom positions [ibid.]

6(h) 6 silicon
6(h) 6 nitrogen
2(c) 2 nitrogen

Polymorphism [ibid.]

A polymorph, α -Si₃N₄ is also hexagonal, with space group P3₁c; its structure has the same tetrahedral units as the β form but their arrangement is different.

Lattice constants

a = 7.608 Å
c = 2.9109
(published values a = 7.608, c = 2.9107 [Hardie and Jack, 1957]).

CD cell; a = 7.608, c = 2.9109, c/a = 0.3826

Volume

145.9 Å³

Density

(measured) 3.19 g/cm³
(calculated) 3.193 g/cm³

Thermal parameters

Isotropic: overall B = 0.5

Scattering factors

Si⁰, N⁰ [International Tables, 1962].

Scale factors (integrated intensities)

$\gamma = 0.457 \times 10^{-3}$

Additional pattern

1. PDF card 9-259 [Decker, General Electric Co., Schenectady, N.Y.]

References

Hardie, D. and Jack, K. H. (1957). Nature, London, No. 4581, Aug. 17, p. 332.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{Å}$
6.58	40	1 0 0	13.44	
3.80	40	1 1 0	23.38	
3.29	100	2 0 0	27.06	
2.66	95	1 0 1	33.64	
2.49	95	2 1 0	36.04	
2.31	6	1 1 1	38.94	
2.20	5	3 0 0	41.08	
2.18	35	2 0 1	41.36	
1.902	8	2 2 0	47.78	
1.892	5	2 1 1	48.04	
1.827	12	1 3 0	49.86	
1.753	35	3 0 1	52.14	
1.592	11	2 2 1	57.86	
1.548	6	1 3 1 ⁺	59.70	
1.511	14	2 3 0 ⁺	61.28	
1.455	14	0 0 2	63.92	
1.438	7	1 4 0 ⁺	64.80	
1.434	6	4 0 1	64.98	
1.359	2	1 1 2	69.04	
1.341	40	2 3 1	70.10	
1.331	8	2 0 2	70.70	
1.318	4	5 0 0	71.54	
1.289	20	4 1 1	73.40	
1.268	6	3 3 0	74.82	
1.257	16	2 1 2	75.62	
1.200	2	5 0 1	79.84	
1.183	1	5 1 0 ⁺	81.22	
1.156	2	2 2 2	83.58	
1.145	3	2 4 1 ⁺	84.58	
1.138	4	1 3 2	85.16	
1.096	4	5 1 1	89.28	
1.083	3	4 3 0	90.66	
1.055	1	2 5 0	93.80	
1.048	7	2 3 2 ⁺	94.58	
1.023	4	1 4 2 ⁺	97.72	
1.015	1	3 4 1	98.72	
1.005	2	1 6 0	100.10	
.9919	3	2 5 1 ⁺	101.90	
.9769	3	5 0 2	104.10	
.9599	3	1 0 3	106.74	
.9560	5	3 3 2	107.36	
.9497	10	1 6 1 ⁺	108.40	
.9413	2	5 3 0	109.84	
.9307	2	2 0 3	111.72	
.9182	2	5 1 2 ⁺	114.06	
.9137	2	2 6 0 ⁺	114.92	
.9040	4	4 4 1	116.88	
.8956	2	7 0 1 ⁺	118.66	

Silicon nitride, β -Si₃N₄ - (Continued)

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å
6.59	35	1 0 0	13.43	
3.80	41	1 1 0	23.37	
3.29	100	2 0 0	27.04	
2.66	100	1 0 1	33.63	
2.49	100	2 1 0	36.04	
2.31	6	1 1 1	38.93	
2.20	3	3 0 0	41.06	
2.18	35	2 0 1	41.36	
1.902	9	2 2 0	47.78	
1.892	5	2 1 1	48.04	
1.827	13	1 3 0	49.86	
1.753	40	3 0 1	52.13	
1.592	13	2 2 1	57.87	
1.548	2	3 1 1	59.70	
1.548	5	1 3 1	59.70	
1.512	7	3 2 0	61.28	
1.512	9	2 3 0	61.28	
1.455	17	0 0 2	63.91	
1.438	4	4 1 0	64.79	
1.438	5	1 4 0	64.79	
1.434	3	4 0 1	65.00	
1.359	3	1 1 2	69.04	
1.341	6	3 2 1	70.09	
1.341	45	2 3 1	70.09	
1.331	9	2 0 2	70.71	
1.318	5	5 0 0	71.54	
1.289	25	4 1 1	73.39	
1.268	7	3 3 0	74.82	
1.257	19	2 1 2	75.62	
1.200	2	5 0 1	79.83	
1.183	2	5 1 0	81.22	
1.156	3	2 2 2	83.59	
1.145	4	2 4 1	84.58	
1.138	4	1 3 2	85.16	
1.096	5	5 1 1	89.28	
1.083	4	4 3 0	90.66	
1.055	1	2 5 0	93.79	
1.048	4	3 2 2	94.57	
1.048	5	2 3 2	94.57	
1.023	3	1 4 2	97.72	
1.023	3	4 1 2	97.72	
1.015	1	3 4 1	98.72	
1.005	3	1 6 0	100.11	
.9919	1	5 2 1	101.90	
.9919	4	2 5 1	101.90	
.9768	5	5 0 2	104.11	
.9599	3	1 0 3	106.74	
.9560	6	3 3 2	107.36	
.9510	1	4 4 0	108.19	
.9498	10	1 6 1	108.39	

Calculated Pattern (Integrated)				
d (Å)	I	hkl	2θ (°)	λ = 1.540598 Å
.9498	4	6 1 1	108.39	
.9412	2	5 3 0	109.85	
.9307	3	2 0 3	111.72	
.9182	2	5 1 2	114.06	
.9137	3	2 6 0	114.93	
.9040	5	4 4 1	116.89	
.8956	1	5 3 1	118.66	
.8956	2	7 0 1	118.66	

Vanadium sulfide, α -V₃S

Structure

Tetragonal, $I\bar{4}2m$ (121), $Z = 8$. The structure was determined by Pedersen and Grønvold [1959], and is closely related to that of Ni₃P.

Atom positions [ibid.]

8(i) 8 vanadium(1) 8(f) 8 vanadium(3)
8(i) 8 vanadium(2) 8(g) 8 sulfur

Polymorphism [ibid.]

The material was stable above 950 °C, and appeared also in samples quenched from 1400 °C. A tetragonal polymorph, β -V₃S is stable below 825 °C, and has the space group $P4_2/nbc$. The structures are closely related.

Lattice constants [ibid.]

$a = 9.470$ Å
 $c = 4.589$

CD cell: $a = 9.470$, $c = 4.589$, $c/a = 0.4846$

Volume
411.6 Å³

Density

(measured) 5.895 g/cm³
(calculated) 5.968 g/cm³

Thermal parameters

$B = 0$ since absorption and temperature effects nearly balance each other [Pedersen and Grønvold, 1959].

Scattering factors

S^0 , V^0 [Cromer polynomial format: Cromer, 1972; Cromer and Mann, 1968].

Scale factors (integrated intensities)

$\gamma = 0.171 \times 10^{-3}$

References

Cromer, D. T. (1972). Private communication.
Cromer, D. T. and Mann, J. B. (1968). Acta Cryst-allogr. A24, 321.
Pedersen, B. and Grønvold, F. (1959). Acta Cryst-allogr. 12, 1022.

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{Å}$
4.13	1	1 0 1	21.52	
3.112	1	2 1 1	28.66	
2.994	1	3 1 0	29.82	
2.601	8	3 0 1	34.46	
2.280	100	3 2 1	39.50	
2.232	55	3 3 0	40.38	
2.170	60	1 1 2	41.58	
2.118	30	4 2 0	42.66	
2.064	20	2 0 2	43.82	
2.054	100	4 1 1	44.06	

Calculated Pattern (Peak heights)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{Å}$
1.892	40	2 2 2	48.04	
1.857	16	5 1 0	49.02	
1.821	12	3 1 2	50.04	
1.751	7	4 3 1 ⁺	52.20	
1.648	9	4 0 2	55.74	
1.643	9	5 2 1	55.92	
1.600	3	3 3 2	57.56	
1.578	1	6 0 0	58.42	
1.497	4	6 2 0	61.92	
1.474	14	6 1 1	63.00	
1.408	1	5 4 1	66.36	
1.376	1	3 0 3	68.06	
1.352	5	4 4 2	69.44	
1.349	6	6 3 1	69.62	
1.339	11	7 1 0 ⁺	70.22	
1.326	9	5 3 2	71.06	
1.322	17	3 2 3	71.28	
1.313	3	6 4 0	71.82	
1.300	10	6 0 2	72.66	
1.2732	15	4 1 3	74.46	
1.2515	10	7 2 1	75.98	
1.2434	5	7 3 0	76.56	
1.1900	2	4 3 3 ⁺	80.68	
1.1722	3	6 5 1	82.16	
1.1566	13	5 5 2	83.52	
1.1472	8	0 0 4	84.36	
1.1378	10	7 4 1	85.22	
1.1160	2	6 6 0	87.30	
1.1010	1	7 5 0	88.80	
1.0911	5	6 1 3	89.82	
1.0774	7	8 3 1	91.28	
1.0521	6	8 0 2	94.14	
1.0374	2	6 3 3	95.90	
1.0269	3	8 2 2	97.20	
1.0257	1	9 0 1	97.36	
1.0203	6	3 3 4	98.04	
1.0133	1	7 0 3	98.96	
1.0087	4	4 2 4	99.58	
1.0023	2	9 2 1 ⁺	100.44	
.9909	5	7 2 3	102.04	
.9806	2	8 5 1	103.54	
.9761	4	5 1 4	104.22	
.9515	3	9 1 2	108.10	
.9502	2	6 5 3	108.32	
.9470	5	10 0 0	108.86	
.9411	6	9 4 1	109.88	
.9317	6	7 4 3	111.54	

Vanadium sulfide, α -V₃S - (Continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{\AA}$
4.13	1	1 0 1	21.50	
3.112	1	2 1 1	28.66	
2.995	1	3 1 0	29.81	
2.601	8	3 0 1	34.46	
2.294	1	0 0 2	39.23	
2.280	100	3 2 1	39.50	
2.232	55	3 3 0	40.38	
2.171	60	1 1 2	41.57	
2.118	30	4 2 0	42.66	
2.065	14	2 0 2	43.81	
2.054	100	4 1 1	44.05	
1.893	40	2 2 2	48.03	
1.857	17	5 1 0	49.01	
1.821	13	3 1 2	50.04	
1.751	3	5 0 1	52.21	
1.751	4	4 3 1	52.21	
1.648	9	4 0 2	55.75	
1.642	6	5 2 1	55.95	
1.600	3	3 3 2	57.56	
1.578	1	6 0 0	58.42	
1.497	4	6 2 0	61.92	
1.474	16	6 1 1	63.00	
1.408	1	5 4 1	66.35	
1.377	1	3 0 3	68.05	
1.352	5	4 4 2	69.44	
1.349	4	6 3 1	69.62	
1.339	7	7 1 0	70.22	
1.339	5	5 5 0	70.22	
1.326	10	5 3 2	71.05	
1.322	14	3 2 3	71.29	
1.313	2	6 4 0	71.83	
1.300	11	6 0 2	72.65	
1.2976	2	7 0 1	72.83	
1.2732	18	4 1 3	74.46	
1.2540	1	6 2 2	75.80	
1.2515	11	7 2 1	75.98	
1.2435	5	7 3 0	76.56	
1.1900	1	5 0 3	80.68	
1.1900	1	4 3 3	80.68	
1.1723	4	6 5 1	82.16	
1.1566	15	5 5 2	83.51	
1.1541	2	5 2 3	83.74	
1.1472	9	0 0 4	84.36	
1.1398	2	6 4 2	85.04	
1.1379	11	7 4 1	85.21	
1.1161	2	6 6 0	87.29	
1.1009	1	7 5 0	88.81	
1.0911	5	6 1 3	89.82	
1.0774	9	8 3 1	91.28	
1.0520	7	8 0 2	94.15	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{\AA}$
1.0374	2	6 3 3	95.89	
1.0270	3	8 2 2	97.19	
1.0256	1	9 0 1	97.37	
1.0204	8	3 3 4	98.04	
1.0134	1	7 0 3	98.95	
1.0087	5	4 2 4	99.57	
1.0024	2	9 2 1	100.44	
1.0024	1	7 6 1	100.44	
.9909	6	7 2 3	102.03	
.9806	2	8 5 1	103.54	
.9760	5	5 1 4	104.22	
.9516	4	9 1 2	108.09	
.9502	2	6 5 3	108.32	
.9470	6	10 0 0	108.86	
.9411	8	9 4 1	109.87	
.9316	8	7 4 3	111.55	

Vanadium sulfide, β -V₃S

Structure

Tetragonal, $P4_2/nbc$ (133), $Z = 8$. The structure was determined by Pedersen and Grønvold [1959] and shows relationship to the β -W structure type.

Atom positions [ibid.]

8(j) 8 vanadium(1) 8(i) 8 vanadium(3)
8(j) 8 vanadium(2) 8(h) 8 sulfur

Polymorphism [ibid.]

The material was stable below 825 °C. A tetragonal polymorph, α -V₃S has the space group $I4_2m$; it is stable above 950 °C and appears also in samples quenched from 1400 °C. The two structures are closely related.

Lattice constants [ibid.]

$a = 9.381$ Å
 $c = 4.663$

CD cell: $a = 9.381$, $c = 4.663$, $c/a = 0.4971$

Volume Å³
410.4

Density

(measured) 5.939 g/cm³
(calculated) 5.985 g/cm³

Thermal parameters

$B = 0$, since absorption and temperature effects nearly balance each other [Pedersen and Grønvold, 1959].

Scattering factors

V^0 , S^0 , [Cromer polynomial format: Cromer, 1972; Cromer and Mann, 1968].

Scale factors (integrated intensities)

$\gamma = 0.152 \times 10^{-3}$

References

Cromer, D. T. (1972). Private communication.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Pedersen, B. and Grønvold, F. (1959). Acta Crystallogr. 12, 1022.

Calculated Pattern (Peak heights)				
d (Å)	I	hkl	2θ (°)	$\lambda = 1.540598\text{Å}$
2.502	25	3 1 1	35.86	
2.345	2	4 0 0	38.36	
2.332	2	0 0 2	38.58	
2.272	100	3 2 1	39.64	
2.211	60	3 3 0	40.78	
2.200	75	1 1 2	41.00	
2.097	45	4 2 0+	43.10	
2.045	75	4 1 1	44.26	
1.913	30	4 2 1	47.50	
1.907	60	2 2 2	47.64	
1.840	20	5 1 0	49.50	
1.834	19	3 1 2	49.68	
1.711	6	5 1 1	53.50	
1.653	9	4 0 2	55.54	
1.605	4	3 3 2	57.38	
1.483	4	6 2 0+	62.58	
1.464	15	6 1 1	63.48	
1.414	1	6 2 1	66.04	
1.398	1	5 4 1	66.88	
1.377	2	3 1 3	68.04	
1.351	4	4 4 2	69.50	
1.339	2	6 3 1	70.22	
1.334	14	3 2 3	70.52	
1.326	13	7 1 0+	71.00	
1.324	14	5 3 2	71.16	
1.2984	14	6 0 2	72.78	
1.2953	10	4 0 3	72.98	
1.2835	12	4 1 3	73.76	
1.2761	3	7 1 1	74.26	
1.2531	9	6 4 1	75.86	
1.2498	7	4 2 3	76.10	
1.2420	6	7 2 1	76.66	
1.2317	5	7 3 0	77.42	
1.1910	7	7 3 1	80.60	
1.1878	5	5 1 3	80.86	
1.1657	9	0 0 4	82.72	
1.1530	15	5 5 2	83.84	
1.1361	2	6 4 2	85.38	
1.1055	2	6 6 0	88.34	
1.0947	5	6 1 3	89.44	
1.0907	1	7 5 0	89.86	
1.0687	8	8 3 1	92.24	
1.0619	5	7 5 1	93.00	
1.0476	6	8 0 2	94.66	
1.0312	7	3 3 4	96.66	
1.0231	4	8 4 1	97.68	
1.0225	4	8 2 2	97.76	
1.0190	6	4 2 4	98.22	
1.0114	2	9 1 1	99.22	
1.0090	2	7 1 3	99.54	

Vanadium sulfide, $\beta\text{-V}_3\text{S}$ - (Continued)

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{\AA}$
2.503	20	3 1 1	35.85	
2.345	2	4 0 0	38.35	
2.331	1	0 0 2	38.58	
2.272	100	3 2 1	39.64	
2.211	55	3 3 0	40.78	
2.200	65	1 1 2	41.00	
2.098	35	4 2 0	43.09	
2.095	16	4 0 1	43.14	
2.088	16	2 0 2	43.30	
2.045	75	4 1 1	44.26	
1.913	20	4 2 1	47.49	
1.907	55	2 2 2	47.64	
1.840	20	5 1 0	49.50	
1.833	13	3 1 2	49.70	
1.711	7	5 1 1	53.50	
1.653	9	4 0 2	55.53	
1.604	5	3 3 2	57.39	
1.483	4	6 2 0	62.57	
1.482	1	6 0 1	62.62	
1.464	17	6 1 1	63.48	
1.413	1	6 2 1	66.04	
1.398	1	5 4 1	66.89	
1.377	3	3 1 3	68.04	
1.351	5	4 4 2	69.50	
1.339	1	6 3 1	70.21	
1.334	15	3 2 3	70.52	
1.327	8	7 1 0	70.99	
1.327	5	5 5 0	70.99	
1.324	10	5 3 2	71.14	
1.301	3	6 4 0	72.62	
1.2985	15	6 0 2	72.77	
1.2956	3	4 0 3	72.96	
1.2834	14	4 1 3	73.77	
1.2760	3	7 1 1	74.27	
1.2531	10	6 4 1	75.87	
1.2515	1	6 2 2	75.98	
1.2488	5	4 2 3	76.17	
1.2420	7	7 2 1	76.66	
1.2318	6	7 3 0	77.42	
1.1909	8	7 3 1	80.60	
1.1873	2	5 1 3	80.90	
1.1657	10	0 0 4	82.72	
1.1531	18	5 5 2	83.83	
1.1360	2	6 4 2	85.38	
1.1056	3	6 6 0	88.33	
1.0948	6	6 1 3	89.44	
1.0905	1	7 5 0	89.88	
1.0687	9	8 3 1	92.23	
1.0619	6	7 5 1	93.01	
1.0476	7	8 0 2	94.67	

Calculated Pattern (Integrated)				
d(Å)	I	hkl	2 θ (°)	$\lambda = 1.540598\text{\AA}$
1.0312	9	3 3 4	96.66	
1.0233	3	8 4 1	97.66	
1.0224	3	8 2 2	97.78	
1.0190	6	4 2 4	98.22	
1.0113	3	9 1 1	99.23	
1.0091	2	7 1 3	99.52	

	Vol. or Sec.	Page		Vol. or Sec.	Page
Aluminum, Al	1	11	Ammonium copper bromide hydrate, (NH ₄) ₂ CuBr ₄ ·2H ₂ O	10m	6
Aluminum antimony, AlSb	4	72	Ammonium copper chloride, NH ₄ CuCl ₃	7m	7
Aluminum bismuth oxide, Al ₄ Bi ₂ O ₉ ..	11m	5	Ammonium copper chloride hydrate, (NH ₄) ₂ CuCl ₄ ·2H ₂ O	12m	6
Aluminum chloride, AlCl ₃	9m	61	Ammonium copper fluoride, NH ₄ CuF ₃ ..	11m	8
Aluminum chloride hydrate (chloraluminite), AlCl ₃ ·6H ₂ O	7	3	Ammonium gallium sulfate hydrate, NH ₄ Ga(SO ₄) ₂ ·12H ₂ O	6	9
Aluminum copper, Al ₄ Cu ₉	11m	79	Ammonium germanium fluoride, (NH ₄) ₂ GeF ₆	6	8
Aluminum fluoride hydroxide silicate, topaz, Al ₂ (F,OH) ₂ SiO ₄	1m	4	Ammonium hydrogen carbonate (teschemacherite), (NH ₄)HCO ₃	9	5
Aluminum lithium, Al ₄ Li ₉	10m	98	Ammonium hydrogen phosphate, NH ₄ H ₂ PO ₄	4	64
Aluminum nickel, AlNi	6m	82	Ammonium iodate, NH ₄ IO ₃	10m	7
Aluminum nitride, AlN	12m	5	Ammonium iodide, NH ₄ I	4	56
Aluminum nitrate hydrate, Al(NO ₃) ₃ ·9H ₂ O	11m	6	Ammonium iridium chloride, (NH ₄) ₂ IrCl ₆	8	6
Aluminum oxide (corundum), α-Al ₂ O ₃ ..	9	3	Ammonium iron chloride hydrate, (NH ₄) ₂ FeCl ₅ ·H ₂ O	14m	7
Aluminum oxide hydrate (boehmite), α-Al ₂ O ₃ ·H ₂ O	3	38	Ammonium iron fluoride, (NH ₄) ₃ FeF ₆ ..	9m	9
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Aluminum phosphate (berlinite), AlPO ₄ (trigonal)	10	3	Ammonium lead chloride, (NH ₄) ₂ PbCl ₆ ..	11m	10
Aluminum phosphate, AlPO ₄ (orthorhombic)	10	4	Ammonium magnesium aluminum fluoride, NH ₄ MgAlF ₆	10m	9
Aluminum silicate (mullite), Al ₆ Si ₂ O ₁₃	3m	3	Ammonium magnesium chromium oxide hydrate, (NH ₄) ₂ Mg(CrO ₄) ₂ ·6H ₂ O	8m	10
Aluminum tungsten oxide, Al ₂ (WO ₄) ₃ ..	11m	7	Ammonium magnesium phosphate hydrate (struvite), MgNH ₄ PO ₄ ·6H ₂ O	3m	41
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Ammonium aluminum selenate hydrate, NH ₄ Al(SeO ₄) ₂ ·12H ₂ O	9m	6	Ammonium manganese(II) fluoride, NH ₄ MnF ₃	5m	8
Ammonium aluminum sulfate, NH ₄ Al(SO ₄) ₂	10m	5	Ammonium manganese sulfate, (NH ₄) ₂ Mn ₂ (SO ₄) ₃	7m	8
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Ammonium chlorate, NH ₄ ClO ₄ (orthorhombic)	7	6	Ammonium palladium chloride, (NH ₄) ₂ PdCl ₆	8	7
Ammonium chloride (sal-ammoniac), NH ₄ Cl	1	59	Ammonium platinum bromide, (NH ₄) ₂ PtBr ₆	9	6
Ammonium chromium sulfate hydrate, NH ₄ Cr(SO ₄) ₂ ·12H ₂ O	6	7	Ammonium platinum chloride, (NH ₄) ₂ PtCl ₆	5	3
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Further work on this program is in progress, and it is anticipated that additional sections will be issued. Therefore, the cumulative index here is not necessarily the concluding index for the project.

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A mineral name in () indicates a synthetic sample.

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Cesium beryllium fluoride, CsBeF_3 ...	9m	69	Cesium vanadium sulfate hydrate, $\text{CsV}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	1m	11
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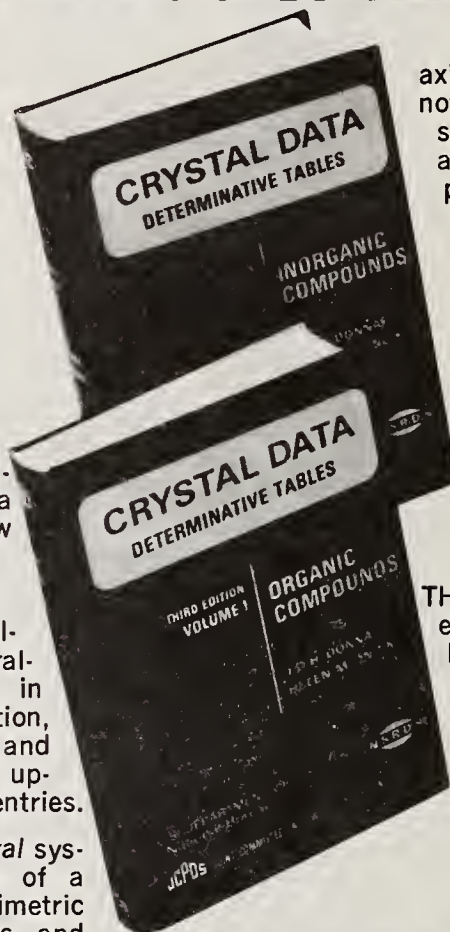
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